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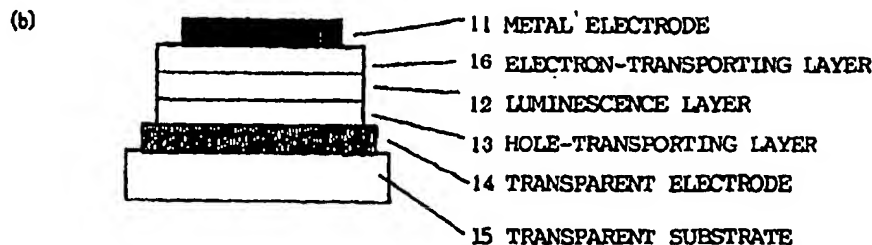
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(54) **LUMINESCENT ELEMENT AND DISPLAY**

(57) In a luminescence device formed of one or plural layers of organic film between a cathode and an anode, at least one layer is a luminescence layer, and a luminescence molecule of a metal coordination compound having a basic structure represented by formula (1) below and having a substituent on at least one of cyclic groups A and B is incorporated as a guest in a host material at a concentration of at least 8 wt. %, which

is higher than a concentration at which a luminescence molecule of a similar structure but having no substituent exhibits a maximum luminescence efficiency to form the luminescence layer. As a result, a high-efficiency luminescence device is provided, which is less liable to cause concentration extinction even when a luminescence molecule is contained at a high concentration relative to the host material in the luminescence layer.

FIG. 1



Description

[TECHNICAL FIELD]

5 [0001] The present invention relates to an organic film luminescence device for use in a planar light source, a planar display, etc.

[0002] The present invention relates to a luminescence device using an organic compound, more particularly to a high-efficiency luminescence device containing in its luminescence layer a luminescence material comprising a metal coordination compound less liable to cause concentration extinction even when used at a high concentration.

[BACKGROUND ART]

10 [0003] An old example of organic luminescence device is, e.g., one using luminescence of a vacuum-deposited anthracene film (Thin Solid Films, 94 (1982) 171). In recent years, however, in view of advantages, such as easiness of providing a large-area device compared with an inorganic luminescence device, and possibility of realizing desired luminescence colors by development of various new materials and drivability at low voltages, an extensive study thereon for device formation as a luminescence device of a high-speed responsiveness and a high efficiency, has been conducted.

15 [0004] As described in detail in, e.g., Macromol. Symp. 125, 1 - 48 (1997), an organic EL device generally has a structure comprising upper and lower two electrodes and a plurality of organic film layers between the electrodes formed on a transparent substrate. Basic structures thereof are shown in Figures 1(a) and (b).

[0005] As shown in Figure 1, an organic EL device generally has a structure comprising a transparent, electrode 14, a metal electrode 11, and a plurality of organic film layers therebetween on a transparent substrate 15.

20 [0006] In the device of Figure 1(a), the organic layers comprise a luminescence layer 12 and a hole-transporting layer 13. For the transparent electrode 14, ITO, etc., having a large work function are used, for providing a good hole-injection characteristic from the transparent electrode 14 to the hole-transporting layer 13. For the metal electrode 11, a metal, such as aluminum, magnesium or an alloy of these, having a small work function is used for providing a good electron-injection characteristic. These electrodes have a thickness of 50 - 200 nm.

25 [0007] For the luminescence layer 12, aluminum quinoxaline complexes (a representative example thereof is Alq3 shown hereinafter), etc., having an electron-transporting characteristic and luminescence characteristic are used. For the hole-transporting layer, biphenyldiamine derivatives (a representative example thereof is α -NPD shown hereinafter), etc., having an electron-donative characteristic are used.

30 [0008] The above-structured device has a rectifying characteristic, and when an electric field is applied between the metal electrode 11 as a cathode and the transparent electrode 14 as an anode, electrons are injected from the metal electrode 11 into the luminescence layer 12 and holes are injected from the transparent electrode 15. The injected holes and electrons are recombined within the luminescence layer 12 to form excitons and cause luminescence. At this time, the hole-transporting layer 13 functions as an electron-blocking layer to increase the recombination efficiency at a boundary between the luminescence layer 12 and hole-transporting layer 13, thereby increasing the luminescence efficiency.

35 [0009] Further, in the structure of Figure 1(b), an electron-transporting layer 16 is disposed between the metal electrode 11 and the luminescence layer 12. By separating the luminescence and the electron and hole-transportation to provide a more effective carrier blocking structure, effective luminescence can be performed. For the electron-transporting layer 16, an electron-transporting material, such as an oxadiazole derivative, is used.

40 [0010] Known luminescence processes used heretofore in organic EL devices include one utilizing an excited singlet state and one utilizing an excited triplet state, and the transition from the former state to the ground state is called "fluorescence" and the transition from the latter state to the ground state is called "phosphorescence". And the substances in these excited states are called a singlet exciton and a triplet exciton, respectively.

45 [0011] In most of the organic luminescence devices studied heretofore, fluorescence caused by the transition from the excited singlet state to the ground state, has been utilized. On the other hand, in recent years, devices utilizing phosphorescence via triplet excitons have been studied.

50 [0012] Representative published literature may include:

Article 1: Improved energy transfer in electrophosphorescent device (D.F. O'Brien, et al., Applied Physics Letters, Vol. 74, No. 3, p. 422 (1999)); and

55 Article 2: Very high-efficiency green organic light-emitting devices based on electrophosphorescence (M.A. Baldo, et al., Applied Physics Letters, Vol. 75, No. 1, p. 4 (1999)).

[0013] In these articles, a structure including 4 organic layers devices as shown in Figure 1(c) has been principally

used, including, from the anode side, a hole-transporting layer 13, a luminescence layer 12, an exciton diffusion-prevention layer 17 and an electron-transporting layer 11. Materials used therein include carrier-transporting materials and phosphorescent materials, of which the names and structures are shown below together with their abbreviations.

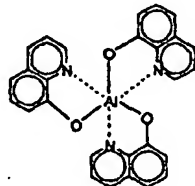
Alq3: aluminum quinolinol complex

α -NPD: N4,N4'-di-naphthalene-1-yl-N4,N4'-diphenyl-biphenyl-4,4'-diamine

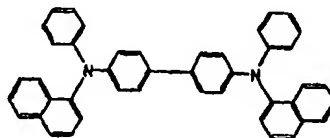
CBP: 2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline

PtOEP: platinum-octaethylporphyrin complex

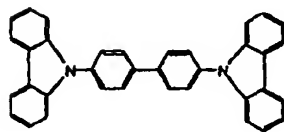
Ir(ppy)₃: iridium-phenylpyrimidine complex



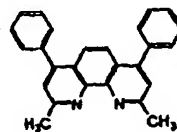
Alq3



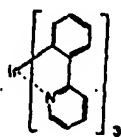
α -NPD



CBP



BCP



Ir(ppy)₃

[0014] The above-mentioned Articles 1 and 2 both have reported structures, as exhibiting a high efficiency, including a hole-transporting layer 13 comprising α -NPD, an electron-transporting layer 16 comprising Alq3, an exciton diffusion-preventing layer 17 comprising BCP, and a luminescence layer 12 comprising CBP as a host and ca. 6 % of platinum-octaethylporphyrin complex (PtOEP) or iridium-phenylpyrimidine complex (Ir(ppy)₃) as a phosphorescent material dispersed in mixture therein.

[0015] Such a phosphorescent material is particularly noted at present because it is expected to provide a high luminescence efficiency in principle for the following reasons. More specifically, excitons formed by carrier recombination comprise singlet excitons and triplet excitons in a probability ratio of 1:3. Conventional organic EL devices have utilized fluorescence of which the luminescence efficiency is limited to at most 25 %. On the other hand, if phosphorescence generated from triplet excitons is utilized, an efficiency of at least three times is expected, and even an efficiency of 100 %, i.e., four times, can be expected in principle, if a transition owing to intersystem crossing from a singlet state having a higher energy to a triplet state is taken into account.

[0016] However, like a fluorescent-type device, such an organic luminescence device utilizing phosphorescence is generally required to be further improved regarding the deterioration of luminescence efficiency and device stability.

[0017] The reason of the deterioration has not been fully clarified, but the present inventors consider as follows based on the mechanism of phosphorescence.

[0018] In the case where the luminescence layer comprises a host material having a carrier-transporting function

and a phosphorescent guest material, a process of phosphorescence via triplet excitons may include unit processes as follows:

1. transportation of electrons and holes within a luminescence layer,
2. formation of host excitons,
3. excitation energy transfer between host molecules,
4. excitation energy transfer from the host to the guest,
5. formation of guest triplet excitons, and
6. transition of the guest triplet excitons to the ground state and phosphorescence.

[0019] Desirable energy transfer in each unit process and luminescence are caused in competition with various energy deactivation processes.

[0020] Particularly, in a phosphorescent material, this may be attributable to a life of the triplet excitons which is longer by three or more digits than the life of a singlet exciton. More specifically, because it is held in a high-energy excited state for a longer period, it is liable to react with surrounding materials and cause polymer formation among the excitons, thus incurring a higher probability of deactivation process resulting in a material change or life deterioration, as we have considered.

[0021] Needless to say, a luminescence efficiency of an organic luminescence device is increased by increasing the luminescence quantum yield of a luminescence center material, but is also an important factor for enhancing the luminescence intensity of the device to increase the concentration of a luminescence material in the luminescence layer.

[0022] The luminescence intensity is increased in proportion to the concentration of a luminescence material in a luminescence layer in the case of a low concentration (up to several wt. %) of the luminescence material in the luminescence layer. However, above several % or 7 %, a deviation from the proportional relationship is observed, and the luminescence intensity is rather lowered to result in a worse efficiency. This phenomenon is reported in Japanese Laid-Open Patent Application (JP-A) 05-078655, JP-A 05-320633, etc., and is known as concentration extinction or concentration deactivation.

[0023] Actually, in the case of using Ir(ppy)₃ in CBP as the host material, the best luminescence efficiency is attained at a concentration of ca. 6 - 7 %, and the luminescence efficiency is rather lowered thereabove, down to about a half at 12 % concentration and 1/10 or below at 100 % concentration (Applied Physics Letters 4, vol. 75, 1999).

[0024] The phenomenon is caused by abundant presence of molecules in the triplet excited state waiting for luminescence in the case of a phosphorescence substance having a life of triplet exciton longer by 3 digits or more than the life of singlet exciton. In this state, thermal deactivation of losing energy due to mutual interaction of triplet excitons is liable to occur. This is called triplet-triplet extinction and is associated with a lowering in luminescence efficiency at a high current density. Further, it is also considered that due to a long retention time at a high energy state, the excitons are caused to have an increased probability of reaction with a surrounding material and formation of polymers of excitons causing deactivation, or even leading to material change or deterioration of life.

[DISCLOSURE OF INVENTION]

[0025] An object of the present invention is to provide an organic luminescence device of a higher luminescence intensity by suppressing the above-mentioned concentration extinction phenomenon and providing an environment of using a luminescence material at a higher concentration.

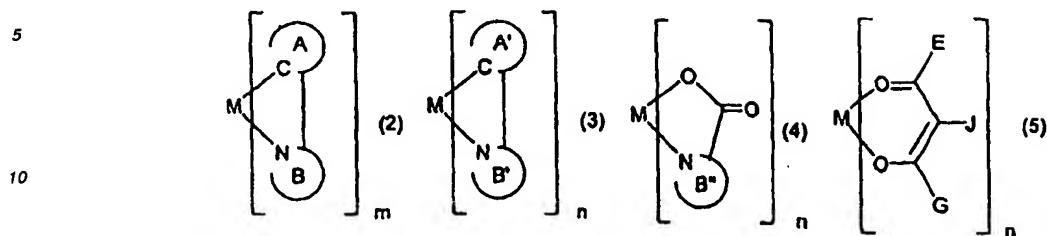
[0026] More specifically, an object of the present invention is to provide a luminescence material less liable to cause concentration extinction even when used at a high concentration with respect to the host material in a luminescence layer by introducing a substituent group into a metal coordination compound as such a luminescence material.

[0027] A more specific object of the present invention is to provide an organic luminescence device capable of a large luminescence intensity, that is an organic luminescence device, comprising: a pair of electrodes each disposed on a substrate, and at least one luminescence layer comprising an organic compound disposed between the electrodes; wherein the luminescence layer comprises a non-luminescent first organic compound and a phosphorescent second organic compound represented by formula (1) shown below, and the second organic compound is present at a concentration of at least 8 wt. % in the luminescence layer:

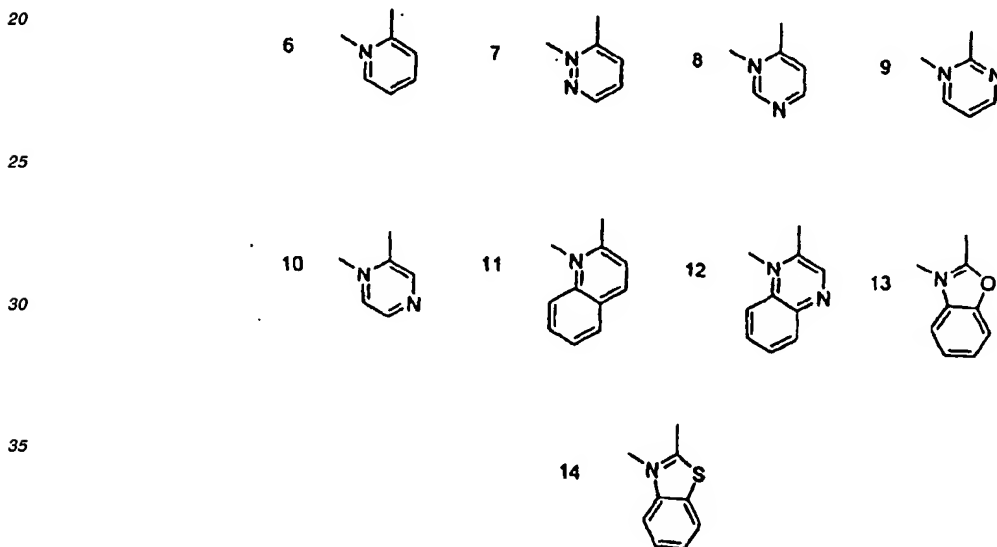


wherein M is a metal atom of Ir, Pt, Rh or Pd; L and L' are mutually different bidentate ligands; m is 1, 2 or 3; n is 0, 1 or 2 with the proviso that m+n is 2 or 3; a partial structure ML_m is represented by formula (2) shown below and a partial

structure ML'_n is represented by formula (3), (4) or (5) shown below:



15 wherein N and C are nitrogen and carbon atoms, respectively; A and A' are respectively a cyclic group capable of having a substituent and bonded to the metal atom M via the carbon atom; B, B' and B'' are respectively a cyclic group represented by a formula of (6) - (14) shown below capable of having a substituent and connected to the metal atom M via the nitrogen atom:



45 **[0028]** According to another aspect, the organic luminescence device of the present invention is a luminescence device comprising one or plural layers of organic film disposed between a cathode and an anode and including at least one layer of luminescence layer, that is characterized by containing a luminescence molecule of the formula (1) having a substituent and showing a maximum luminescence characteristic at a concentration higher than a concentration at which a luminescence molecule of a similar structure but having no substituent shows a maximum luminescence efficiency.

50 **[0029]** More specifically, in a luminescence device comprising one or plural layers of organic film between a cathode and an anode, including at least one layer of luminescence layer, it is preferred that a luminescence molecule of the formula (1) including at least one cyclic group having a substituent is contained at a concentration higher than a concentration at which a luminescence molecule of a similar structure shows a maximum luminescence efficiency.

[BRIEF DESCRIPTION OF THE DRAWINGS]

[0030]

55 Figure 1 illustrates embodiments of the luminescence device according to the present invention.
Figure 2 illustrates a simple matrix-type organic EL device according to Example 28.
Figure 3 illustrates drive signals used in Example 28.

Figure 4 schematically illustrates a panel structure including an EL device and drive means.

Figure 5 illustrates an example of pixel circuit.

Figure 6 is a schematic view showing an example of sectional structure of a TFT substrate.

5 [BEST MODE FOR PRACTICING THE INVENTION]

[0031] Basic device structures according to the present invention are similar to those shown in Figures 1(a), (b) and (c).

10 [0032] More specifically, as shown in Figure 1, an organic luminescence device generally comprises, on a transparent electrode 15, a 50 to 200 nm-thick transparent electrode 14, a plurality of organic film layers and a 10 to 500 nm-thick metal electrode 11 formed so as to sandwich the organic layers.

15 [0033] Figure 1(a) shows an embodiment wherein the organic luminescence device comprises a luminescence layer 12 and a hole-transporting layer 13. The transparent electrode 14 may comprise ITO, etc., having a large work function so as to facilitate hole injection from the transparent electrode 14 to the hole-transporting layer 13. The metal electrode 11 comprises a metal material having a small work function, such as aluminum, magnesium or alloys of these elements, so as to facilitate electron injection into the organic luminescence device.

[0034] The luminescence layer 12 comprises a compound according to the present invention. The hole-transporting layer 13 may comprise, e.g., a triphenylamine derivative, as represented by α -NPD mentioned above, and also a material having an electron-donative property as desired.

20 [0035] A device organized above exhibits a current-rectifying characteristic, and when an electric field is applied between the metal electrode 11 as a cathode and the transparent electrode 14 as an anode, electrons are injected from the metal electrode 11 into the luminescence layer 12, and holes are injected from the transparent electrode 15. The injected holes and electrons are recombined in the luminescence layer 12 to form excitons, which cause luminescence. In this instance, the hole-transporting layer 13 functions as an electron-blocking layer to increase the recombination efficiency at the boundary between the luminescence layer 12 and the hole-transporting layer 13, thereby providing an enhanced luminescence efficiency.

25 [0036] Further, in the structure of Figure 1(b), an electron-transporting layer 16 is disposed between the metal electrode 11 and the luminescence layer 12 in Figure 1(a). As a result, the luminescence function is separated from the functions of electron transportation and hole transportation to provide a structure exhibiting more effective carrier blocking, thus increasing the luminescence efficiency. The electron-transporting layer 16, may comprise, e.g., an oxadiazole derivative.

[0037] Figure 1(c) shows another desirable form of a four-layer structure, including a hole-transporting layer 13, a luminescence layer 12, an exciton diffusion prevention layer 17 and an electron-transporting layer 16, successively from the side of the transparent electrode 14 as an anode.

35 [0038] Each of the organic film layers 12, 13, 16 and 17 is formed in a thickness of at most 200 nm, and particularly the luminescence layer 12 is formed in a thickness of 5 - 200 nm.

[0039] The present inventors have got a knowledge that the use of a metal coordination compound including a substituted cyclic group and represented by the above-mentioned formula (1) allows a high efficiency luminescence and provides less liability of concentration extinction even at a high concentration than the conventional level due to suppression of inter-molecular interaction.

40 [0040] It has been also found that the suppression of concentration extinction is an effect attributable to a substituent possessed by the metal coordination compound, and the concentration extinction becomes less liable to occur not regardless of the coordination number of ligands but owing to the presence of a substituent on at least one ligand.

45 [0041] Particularly, as a result, in a conventional phosphorescence-type organic EL device, the luminescence material can be used at a high concentration of 8 % or higher in the luminescence layer, thereby providing an organic EL device exhibiting a high luminescence luminance.

[0042] The metal coordination compound used in the present invention emits phosphorescence, and its lowest excited state is believed to be an MLCT* (metal-to-ligand charge transfer) excited state or π - π * excited state in a triplet state, and phosphorescence is caused at the time of transition from such a state to the ground state.

50 [0043] It is generally said that phosphorescence life is shorter at MLCT* than at π - π *, but the molecular structure suppressing the concentration used in the present invention is effective for both MLCT* and π - π * as the lowest excited state, and the molecule can be doped at a high concentration in the luminescence layer in either case.

55 [0044] The luminescence material of the present invention exhibited a high phosphorescence yield of from 0.1 to 0.9 and a short phosphorescence life of 0.1 - 30 μ sec. The phosphorescence yield referred to herein is a relative quantum yield, i.e., a ratio of an objective sample's quantum yield ϕ (sample) to a standard sample's quantum yield ϕ (st)) and is determined according to the following formula:

$$\phi(\text{sample})/\phi(\text{st}) = \frac{[\text{Sem}(\text{sample})/\text{Iabs}(\text{sample})]}{[\text{Sem}(\text{st})/\text{Iabs}(\text{st})]},$$

wherein Iabs(st) denotes an absorption coefficient at an excitation wavelength of the standard sample; Sem(st), a luminescence spectral areal intensity when excited at the same wavelength; Iabs(sample), an absorption coefficient at an excitation wavelength of an objective compound; and Sem(sample), a luminescence spectral areal intensity when excited at the same wavelength.

[0045] Phosphorescence yield values described herein are relative values with respect to a phosphorescence yield $\phi = 1$ of Ir(ppy)₃ as a standard sample.

[0046] Further, the luminescence (phosphorescence) life referred to herein is based on values measured according to the following method.

<<Method of measurement of life>>

[0047] A sample compound is dissolved in chloroform and spin-coated onto a quartz substrate in a thickness of ca. 0.1 μm and is exposed to pulsative nitrogen laser light at an excitation wavelength of 337 nm at room temperature by using a luminescence life meter (made by Hamamatsu Photonics K.K.). After completion of the excitation pulses, the decay characteristic of luminescence intensity is measured.

[0048] When an initial luminescence intensity is denoted by I_0 , a luminescence intensity after $t(\text{sec})$ is expressed according to the following formula with reference to a luminescence life $\tau(\text{sec})$:

$$I = I_0 \cdot \exp(-t/\tau).$$

[0049] Thus, the luminescence life τ is a time period in which the luminescence intensity I is attenuated down to $1/e$ of the initial intensity I ($I/I_0 = e^{-1}$, e is a base of natural logarithm).

[0050] A short phosphorescence life is a condition for providing an EL device of a high luminescence efficiency. More specifically, a long phosphorescence life means abundant presence of molecules in a triplet excited state waiting for the luminescence leading to a problem of a lowering in luminescence efficiency particularly at a high current density. The material of the present invention is a suitable luminescence material for an EL device because of a high phosphorescence yield and a short phosphorescence life. Further, it is assumed that because of a short phosphorescence life, the duration at a triplet state is shortened to suppress the concentration extinction. A high stability of the luminescence material of the present invention was also exhibited in an actual current conduction test of actual devices.

[0051] In the case of a phosphorescent material, the luminescence characteristic thereof is severely affected by its molecular environment. In the case of a fluorescence device, the basic property of a luminescence material is examined based on photoluminescence. In the case of phosphorescence, however, the photoluminescence performance does not directly lead to the luminescence performance of an EL device since it is frequently affected by the polarity of host molecules, temperature and solid/liquid state. As a result, EL device performances except for a part thereof cannot be estimated from the photoluminescence result.

[0052] In the case of a ligand of the present invention having a cyclic group having one or plural fluorine atoms, it becomes possible to shift the luminescence wavelength to a shorter side or a longer side because of a change in energy gap. If it is assumed for convenience that HOMO/LUMO of metal electron orbits and HOMO/LUMO of ligand electron orbits can be considered separately, it is understood that MOHO/LUMO energy levels of ligand electron orbits are changed by fluorine atoms having a large electronegativity to change the energy gap between the HOMO level of the metal and the LUMO level of the ligand, thereby shifting the luminescence from the MCLT state as the lowest excited state to a shorter wavelength side or a longer wavelength side. Accordingly, while a luminescence material exhibiting a stably high quantum yield over a broad wavelength range (blue to red) has not been found, it can be realized by a luminescence material of the present invention, thus being able to provide a luminescence material which shows a high efficiency at a desired emission wavelength over a board wavelength range (from blue to red).

[0053] When a device is formed, due to a large electronegativity of fluorine atoms, the inter-molecular interaction is suppressed to physically result in a suppressed crystallinity favoring a uniform film formation and physically suppressing the dimerization reaction to prohibit the energy deactivation leading to an improved luminescence efficiency, thus resulting in an improved electrical property and an improved device stability.

[0054] Further, in the case of using a ligand containing a plurality of fluorine atoms or polyfluoroalkyl groups as substituents, it is considered that direct interaction between luminescence molecules is suppressed due to electrical repulsion caused by their electrical effect or due to steric hindrance, thereby preventing energy deactivation and con-

centration extinction.

[0055] Further, from the viewpoint of device preparation, a luminescence material having a substituent, particularly a fluorinated substituent, allows easier vacuum deposition due to a lowering in sublimation temperature. In the film formation by vacuum deposition, thus providing a great advantage also in this respect.

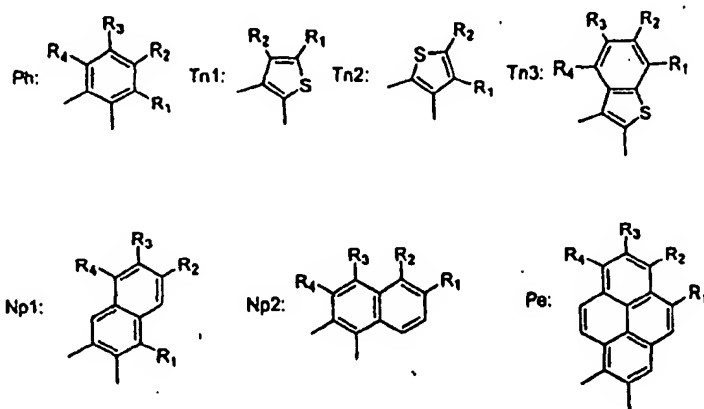
[0056] As a result, as shown in Examples described hereinafter, by using a luminescence material having a substituent according to the present invention, a stable luminescence for long hours with suppressed concentration extinction can be expected. Further, it becomes possible to attain a high phosphorescence yield over a temperature range of from -20 °C to 60 °C as an actual operation temperature range of an organic luminescence device. Further, in the case of using a compound at a concentration of 8 wt. % or higher with respect to a host material in the luminescence layer or at a concentration higher than a compound having no substituent, it becomes possible to provide an EL device exhibiting excellent luminescence performance while suppressing the concentration extinction. The concentration of the luminescence material of the present invention in the luminescence layer may be at least 8 wt. %, preferably 10 wt. % or higher, but the luminescence material potentially has a possibility of being used even at 100 % without causing substantial concentration extinction.

[0057] Herein, the term "luminescence performance" refers to a characteristic attributable to a maximum luminescence efficiency which can be expressed as any of a maximum luminance, a maximum of luminance/current, a maximum of light flux/power consumption or a maximum of external quantum yield.

[0058] A high-efficiency luminescence device according to the present invention is applicable to a product requiring energy economization or a high luminance. More specifically, the luminescence device is applicable to a display apparatus, an illumination apparatus, a printer light source or a backlight for a luminescence layer display apparatus. As for a display apparatus, it allows a flat panel display which is light in weight and provides a highly recognizable display at a low energy consumption. As a printer light source, the luminescence device of the present invention can be used instead of a laser light source of a laser beam printer. Independently addressable devices are arranged in an array form to effect a desired exposure on a photosensitive drum thereby forming an image. The apparatus volume can be remarkably reduced by using the devices of the present invention. For the illumination apparatus or backlight, the energy economization effect according to the present invention can be expected.

[0059] For the application to a display, a drive system using a thin-film transistor (abbreviated as TFT) drive circuit according to an active matrix-scheme, may be used. By driving a display panel using a luminescence material of the present invention in a luminescence layer, it becomes possible to allow a stable display for long hours at a good picture quality.

[0060] Hereinbelow, some specific structural formulae of metal coordination compounds represented by the formula (1) used in the present invention are shown in Table 1 appearing hereinafter, which are however only representative examples and are not exhaustive. Ph - P9 used in Table 1 represent partial structured shown below, of which substituents R1, R2, ... are shown as A-R1, A-R2, ... when contained in the cyclic group A in the formula (1) and as B-R1, B-R2, ... when contained in the cyclic group B, ... in Table 1.



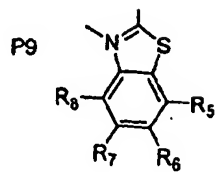
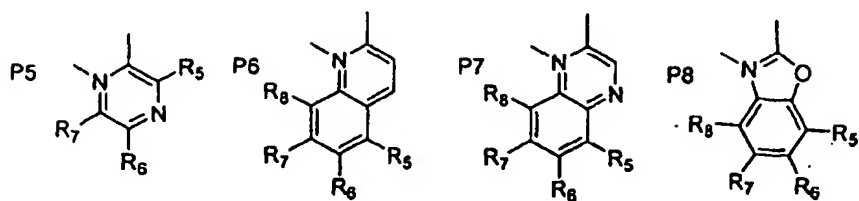
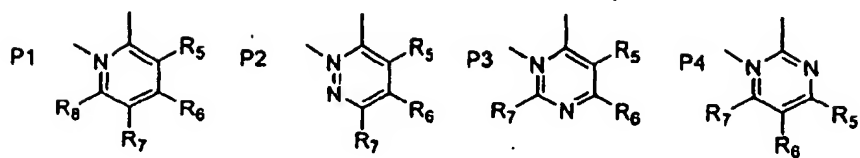
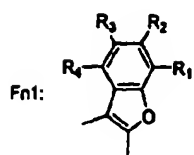
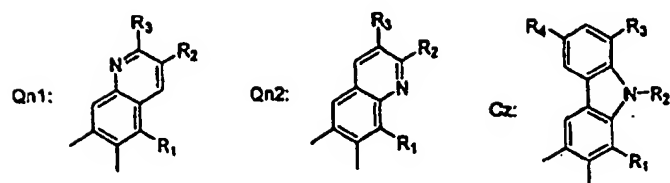
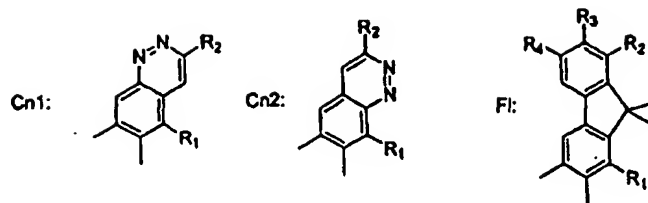


Table 1-1




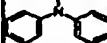
No	M	m	n	A	B	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
1	Ir	3	0	Ph	P1	CH3	H	H	H	H	H	H	H
2	Ir	3	0	Ph	P1	H	CH3	H	H	H	H	H	H
3	Ir	3	0	Ph	P1	H	H	CH3	H	H	H	H	H
4	Ir	3	0	Ph	P1	H	H	H	CH3	H	H	H	H
5	Ir	3	0	Ph	P1	C2H5	H	H	H	H	H	H	H
6	Ir	3	0	Ph	P1	H	C2H5	H	H	H	H	H	H
7	Ir	3	0	Ph	P1	H	H	C2H5	H	H	H	H	H
8	Ir	3	0	Ph	P1	H	H	H	C2H5	H	H	H	H
9	Ir	3	0	Ph	P1	C3H7	H	H	H	H	H	H	H
10	Ir	3	0	Ph	P1	H	C3H7	H	H	H	H	H	H
11	Ir	3	0	Ph	P1	H	H	C3H7	H	H	H	H	H
12	Ir	3	0	Ph	P1	H	H	H	C3H7	H	H	H	H
13	Ir	3	0	Ph	P1	C4H9	H	H	H	H	H	H	H
14	Ir	3	0	Ph	P1	H	C4H9	H	H	H	H	H	H
15	Ir	3	0	Ph	P1	H	H	C4H9	H	H	H	H	H
16	Ir	3	0	Ph	P1	H	H	H	C4H9	H	H	H	H
17	Ir	3	0	Ph	P1	C8H13	H	H	H	H	H	H	H
18	Ir	3	0	Ph	P1	-	C8H13	H	H	H	H	H	H
19	Ir	3	0	Ph	P1	H	H	C8H13	H	H	H	H	H
20	Ir	3	0	Ph	P1	H	H	H	C8H13	H	H	H	H
21	Ir	3	0	Ph	P1	C8H17	H	H	H	H	H	H	H
22	Ir	3	0	Ph	P1	H	C8H17	H	H	H	H	H	H
23	Ir	3	0	Ph	P1	H	H	C8H17	H	H	H	H	H
24	Ir	3	0	Ph	P1	H	H	H	C8H17	H	H	H	H
25	Ir	3	0	Ph	P1	C12H25	H	H	H	H	H	H	H
26	Ir	3	0	Ph	P1	H	C12H25	H	H	H	H	H	H
27	Ir	3	0	Ph	P1	H	H	C12H25	H	H	H	H	H
28	Ir	3	0	Ph	P1	H	H	H	C12H25	H	H	H	H
29	Ir	3	0	Ph	P1	C15H31	H	H	H	H	H	H	H
30	Ir	3	0	Ph	P1	H	C15H31	H	H	H	H	H	H
31	Ir	3	0	Ph	P1	H	H	C15H31	H	H	H	H	H
32	Ir	3	0	Ph	P1	H	H	CH30	H	H	H	H	H
33	Ir	3	0	Ph	P1	H	H	C2H50	H	H	H	H	H
34	Ir	3	0	Ph	P1	H	H	C4H80	H	H	H	H	H
35	Ir	3	0	Ph	P1	H	C4H90	H	H	H	H	H	H
36	Ir	3	0	Ph	P1	H		H	H	H	H	H	H
37	Ir	3	0	Ph	P1	H		H	H	H	H	H	H
38	Ir	3	0	Ph	P1	H	H		H	H	H	H	H
39	Ir	3	0	Ph	P1	H	H		H	H	H	H	H
40	Ir	3	0	Ph	P1	H	H	CF30	H	H	H	H	H
41	Ir	3	0	Ph	P1	H	H	C4F9	H	H	H	H	H
42	Ir	3	0	Ph	P1	H	C4F9	H	H	H	H	H	H
43	Ir	3	0	Ph	P1	H	H	C2F5C2H20	H	H	H	H	H
44	Ir	3	0	Ph	P1	H	C2F5	H	H	H	H	H	H
45	Ir	3	0	Ph	P1	H	H	C2F5	H	H	H	H	H
46	Ir	3	0	Ph	P1	H	H	C3F11	H	H	H	H	H
47	Ir	3	0	Ph	P1	H	H	C8F17	H	H	H	H	H
48	Ir	3	0	Ph	P1	H	H	C2F5C2H4	H	H	H	H	H
49	Ir	3	0	Ph	P1	CH3	H	CH3	H	H	H	H	H
50	Ir	3	0	Ph	P1	H	CH3	CH3	H	H	H	H	H
51	Ir	3	0	Ph	P1	C2H5	H	C2H5	H	H	H	H	H
52	Ir	3	0	Ph	P1	C4H9	H	C4H9	H	H	H	H	H
53	Ir	3	0	Ph	P1	H	C4H9	H	H	H	H	H	H
54	Ir	3	0	Ph	P1	H	H	H	CH3	H	H	H	H
55	Ir	3	0	Ph	P1	H	H	H	H	CH3	H	H	H
56	Ir	3	0	Ph	P1	H	H	H	H	H	CH3	H	H
57	Ir	3	0	Ph	P1	H	H	H	H	H	H	CH3	H
58	Ir	3	0	Ph	P1	H	H	H	H	C4H9	H	H	H
59	Ir	3	0	Ph	P1	H	H	H	H	H	C4H9	H	H
60	Ir	3	0	Ph	P1	H	H	H	H	H	H	C4H9	H

Table 1-2

No	M	m	n	A	B	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
61	Ir	3	0	Ph	P1	H	H	H	H	H	H	H	C4H9
62	Ir	3	0	Ph	P1	H	H	H	H	C8H17	H	H	H
63	Ir	3	0	Ph	P1	H	H	H	H	H	C8H17	H	H
64	Ir	3	0	Ph	P1	H	H	H	H	H	H	C8H17	H
65	Ir	3	0	Ph	P1	H	H	H	H	H	H	H	C8H17
66	Ir	3	0	Ph	P1	CH3	H	H	H	CH3	H	H	H
67	Ir	3	0	Ph	P1	CH3	H	H	H	H	CH3	H	H
68	Ir	3	0	Ph	P1	CH3	H	H	H	H	H	CH3	H
69	Ir	3	0	Ph	P1	CH3	H	H	H	H	H	H	CH3
70	Ir	3	0	Ph	P1	H	CH3	H	H	CH3	H	H	H
71	Ir	3	0	Ph	P1	H	CH3	H	H	H	CH3	H	H
72	Ir	3	0	Ph	P1	H	CH3	H	H	H	H	CH3	H
73	Ir	3	0	Ph	P1	H	CH3	H	H	H	H	H	CH3
74	Ir	3	0	Ph	P1	H	H	CH3	H	CH3	H	H	H
75	Ir	3	0	Ph	P1	H	H	CH3	H	H	CH3	H	H
76	Ir	3	0	Ph	P1	H	H	CH3	H	H	H	CH3	H
77	Ir	3	0	Ph	P1	H	H	CH3	H	H	H	H	CH3
78	Ir	3	0	Ph	P1	H	H	H	CH3	H	H	CH3	H
79	Ir	3	0	Ph	P1	C2H5	H	H	H	H	CH3	H	H
80	Ir	3	0	Ph	P1	C2H5	H	H	H	H	H	CH3	H
81	Ir	3	0	Ph	P1	H	C2H5	H	H	CH3	H	H	H
82	Ir	3	0	Ph	P1	H	C2H5	H	H	H	CH3	H	H
83	Ir	3	0	Ph	P1	H	C2H5	H	H	H	H	CH3	H
84	Ir	3	0	Ph	P1	H	C2H5	H	H	H	H	H	CH3
85	Ir	3	0	Ph	P1	H	H	C2H5	H	CH3	H	H	H

Table 1-2 (continued)

No	M	m	n	A	B	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
86	Ir	3	0	Ph	P1	H	H	C2H5	H	H	CH3	H	H
87	Ir	3	0	Ph	P1	H	H	C2H5	H	H	H	CH3	H
88	Ir	3	0	Ph	P1	H	H	C2H5	H	H	H	H	CH3
89	Ir	3	0	Ph	P1	H	H	H	C2H5	H	CH3	H	H
90	Ir	3	0	Ph	P1	H	H	H	C2H5	H	H	CH3	H
91	Ir	3	0	Ph	P1	C4H9	H	H	H	H	CH3	H	H
92	Ir	3	0	Ph	P1	H	C4H9	H	H	CH3	H	H	H
93	Ir	3	0	Ph	P1	H	C4H9	H	H	H	CH3	H	H
94	Ir	3	0	Ph	P1	H	C4H9	H	H	H	H	CH3	H
95	Ir	3	0	Ph	P1	H	C4H9	H	H	H	H	H	CH3
96	Ir	3	0	Ph	P1	H	H	C4H9	H	H	CH3	H	H
97	Ir	3	0	Ph	P1	H	H	C4H9	H	H	H	CH3	H
98	Ir	3	0	Ph	P1	H	H	H	C4H9	H	CH3	H	H
99	Ir	3	0	Ph	P1	H	H	H	C4H9	H	CH3	H	H
100	Ir	3	0	Ph	P1	C6H13	H	H	H	H	CH3	H	H
101	Ir	3	0	Ph	P1	H	C6H13	H	H	CH3	H	H	H
102	Ir	3	0	Ph	P1	H	C6H13	H	H	H	CH3	H	H
103	Ir	3	0	Ph	P1	H	C6H13	H	H	H	H	CH3	H
104	Ir	3	0	Ph	P1	H	C6H13	H	H	H	H	H	CH3
105	Ir	3	0	Ph	P1	H	H	C6H13	H	H	CH3	H	H
106	Ir	3	0	Ph	P1	H	H	C6H13	H	H	H	CH3	H
107	Ir	3	0	Ph	P1	H	H	H	C6H13	H	CH3	H	H
108	Ir	3	0	Ph	P1	H	H	H	C6H13	H	CH3	H	H
109	Ir	3	0	Ph	P1	CH3	H	H	H	CF3	H	H	H
110	Ir	3	0	Ph	P1	H	CH3	H	H	CF3	H	H	H

Table 1-2 (continued)

No	M	m	n	A	B	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
111	Ir	3	0	Ph	P1	H	H	CH3	H	CF3	H	H	H
112	Ir	3	0	Ph	P1	H	H	H	CH3	CF3	H	H	H
113	Ir	3	0	Ph	P1	CH3	H	H	H	H	CF3	H	H
114	Ir	3	0	Ph	P1	H	CH3	H	H	H	CF3	H	H
115	Ir	3	0	Ph	P1	H	H	CH3	H	H	CF3	H	H
116	Ir	3	0	Ph	P1	H	H	H	CH3	H	CF3	H	H
117	Ir	3	0	Ph	P1	CH3	H	H	H	H	H	CF3	H
118	Ir	3	0	Ph	P1	H	CH3	H	H	H	H	CF3	H
119	Ir	3	0	Ph	P1	H	H	CH3	H	H	H	CF3	H
120	Ir	3	0	Ph	P1	H	H	H	CH3	H	H	CF3	H

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Table 1-3

	No	M	m	n	A	B	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
5	121	lr	3	0	Ph	P1	CH3	H	H	H	H	H	H	CF3
	122	lr	3	0	Ph	P1	H	CH3	H	H	H	H	H	CF3
	123	lf	3	0	Ph	P1	H	H	CH3	H	H	H	H	CF3
	124	lr	3	0	Ph	P1	H	H	H	CH3	H	H	H	CF3
10	125	lr	3	0	Ph	P1	CH3	H	H	H	F	H	H	H
	126	lr	3	0	Ph	P1	H	CH3	H	H	F	H	H	H
	127	lr	3	0	Ph	P1	H	H	CH3	H	F	H	H	H
15	128	lr	3	0	Ph	P1	H	H	H	CH3	F	H	H	H
	129	lr	3	0	Ph	P1	CH3	H	H	H	H	F	H	H
	130	lr	3	0	Ph	P1	H	CH3	H	H	H	F	H	H
20	131	lr	3	0	Ph	P1	H	H	CH3	H	H	F	H	H
	132	lr	3	0	Ph	P1	H	H	H	CH3	H	F	H	H
	133	lr	3	0	Ph	P1	CH3	H	H	H	H	H	F	H
	134	lr	3	0	Ph	P1	H	CH3	H	H	H	H	F	H
25	135	lr	3	0	Ph	P1	H	H	CH3	H	H	H	F	H
	136	lr	3	0	Ph	P1	H	H	H	CH3	H	H	F	H
	137	lr	3	0	Ph	P1	CH3	H	H	H	H	H	H	F
30	138	lr	3	0	Ph	P1	H	CH3	H	H	H	H	H	F
	139	lr	3	0	Ph	P1	H	H	CH3	H	H	H	H	F
	140	lr	3	0	Ph	P1	H	H	H	CH3	H	H	H	F
	141	lr	3	0	Ph	P1	C2H5	H	H	H	CF3	H	H	H
35	142	lr	3	0	Ph	P1	H	C2H5	H	H	CF3	H	H	H
	143	lr	3	0	Ph	P1	H	H	C2H5	H	CF3	H	H	H
	144	lr	3	0	Ph	P1	H	H	H	C2H5	CF3	H	H	H
40	145	lr	3	0	Ph	P1	C2H5	H	H	H	H	CF3	H	H
	146	lr	3	0	Ph	P1	H	C2H5	H	H	H	CF3	H	H
	147	lr	3	0	Ph	P1	H	H	C2H5	H	H	CF3	H	H
	148	lr	3	0	Ph	P1	H	H	H	C2H5	H	CF3	H	H
45	149	lr	3	0	Ph	P1	C2H5	H	H	H	H	H	CF3	H
	150	lr	3	0	Ph	P1	H	C2H5	H	H	H	H	CF3	H
	151	lr	3	0	Ph	P1	H	H	C2H5	H	H	H	CF3	H
50	152	lr	3	0	Ph	P1	H	H	H	C2H5	H	H	CF3	H
	153	lr	3	0	Ph	P1	C2H5	H	H	H	H	H	H	CF3
	154	lr	3	0	Ph	P1	H	C2H5	H	H	H	H	H	CF3
	155	lr	3	0	Ph	P1	H	H	C2HS	H	H	H	H	CF3
55	156	lr	3	0	Ph	P1	H	H	H	C2H5	H	H	H	CF3
	157	lr	3	0	Ph	P1	C2H5	H	H	H	F	H	H	H

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Table 1-3 (continued)

No	M	m	n	A	B	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
5	158	Ir	3	0	Ph	P1	H	C2H5	H	H	F	H	H
	159	Ir	3	0	Ph	P1	H	H	C2H5	H	F	H	H
	160	Ir	3	0	Ph	P1	H	H	H	C2H5	F	H	H
	161	Ir	3	0	Ph	P1	C2H5	H	H	H	H	F	H
10	162	Ir	3	0	Ph	P1	H	C2H5	H	H	H	F	H
	163	Ir	3	0	Ph	P1	H	H	C2H5	H	H	F	H
	164	Ir	3	0	Ph	P1	H	H	H	C2H5	H	F	H
	165	Ir	3	0	Ph	P1	C2H5	H	H	H	H	H	F
15	166	Ir	3	0	Ph	P1	H	C2H5	H	H	H	H	F
	167	Ir	3	0	Ph	P1	H	H	C2H5	H	H	H	F
	168	Ir	3	0	Ph	P1	H	H	H	C2H5	H	H	F
20	169	Ir	3	0	Ph	P1	C2H5	H	H	H	H	H	F
	170	Ir	3	0	Ph	P1	H	C2H5	H	H	H	H	F
	171	Ir	3	0	Ph	P1	H	H	C2H5	H	H	H	F
	172	Ir	3	0	Ph	P1	H	H	H	C2H5	H	H	F
25	173	Ir	3	0	Ph	P1	C4H9	H	H	H	F	H	H
	174	Ir	3	0	Ph	P1	H	C4H9	H	H	F	H	H
	175	Ir	3	0	Ph	P1	H	H	C4H9	H	F	H	H
30	176	Ir	3	0	Ph	P1	H	H	H	C4H9	F	H	H
	177	Ir	3	0	Ph	P1	C4H9	H	H	H	H	F	H
	178	Ir	3	0	Ph	P1	H	C4H9	H	H	H	F	H
	179	Ir	3	0	Ph	P1	H	H	C4H9	H	H	F	H
35	180	Ir	3	0	Ph	P1	H	H	H	C4H8	H	F	H

Table 1-4

No	M	m	n	A	B	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
40	181	Ir	3	0	Ph	P1	C4H9	H	H	H	H	H	F
	182	Ir	3	0	Ph	P1	H	C4H9	H	H	H	F	H
45	183	Ir	3	0	Ph	P1	H	H	C4H9	H	H	H	F
	184	Ir	3	0	Ph	P1	H	H	H	C4H9	H	H	F
	185	Ir	3	0	Ph	P1	C4H9	H	H	H	H	H	F
	186	Ir	3	0	Ph	P1	H	C4H9	H	H	H	H	F
50	187	Ir	3	0	Ph	P1	H	H	C4H9	H	H	H	F
	188	Ir	3	0	Ph	P1	H	H	H	C4H9	H	H	F
	189	Ir	3	0	Ph	P1	C4H9	H	H	H	CF3	H	H
55	190	Ir	3	0	Ph	P1	H	C4H9	H	H	CF3	H	H
	191	Ir	3	0	Ph	P1	H	H	C4H9	H	CF3	H	H
	192	Ir	3	0	Ph	P1	H	H	H	C4H9	CF3	H	H

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Table 1-4 (continued)

	No	M	m	n	A	B	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
5	193	Ir	3	0	Ph	P1	C4H9	H	H	H	H	CF3	H	H
	194	Ir	3	0	Ph	P1	H	C4H9	H	H	H	CF3	H	H
	195	Ir	3	0	Ph	P1	H	H	C4H9	H	H	CF3	H	H
	196	Ir	3	0	Ph	P1	H	H	H	C4H9	H	CF3	H	H
10	197	Ir	3	0	Ph	P1	C4H9	H	H	H	H	H	CF3	H
	198	Ir	3	0	Ph	P1	H	C4H9	H	H	H	H	CF3	H
	199	Ir	3	0	Ph	P1	H	H	C4H9	H	H	H	CF3	H
	200	Ir	3	0	Ph	P1	H	H	H	C4H9	H	H	CF3	H
15	201	Ir	3	0	Ph	P1	C4H9	H	H	H	H	H	H	CF3
	202	Ir	3	0	Ph	P1	H	C4H9	H	H	H	H	H	CF3
	203	Ir	3	0	Ph	P1	H	H	C4H9	H	H	H	H	CF3
20	204	Ir	3	0	Ph	P1	H	H	H	C4H9	H	H	H	CF3
	205	Ir	3	0	Ph	P1	C8H17	H	H	H	F	H	H	H
	206	Ir	3	0	Ph	P1	H	C8H17	H	H	F	H	H	H
	207	Ir	3	0	Ph	P1	H	H	C8H17	H	F	H	H	H
25	208	Ir	3	0	Ph	P1	H	H	H	C8H17	F	H	H	H
	209	Ir	3	0	Ph	P1	C8H17	H	H	H	H	F	H	H
	210	Ir	3	0	Ph	P1	H	C8H17	H	H	H	F	H	H
30	211	Ir	3	0	Ph	P1	H	H	C8H17	H	H	F	H	H
	212	Ir	3	0	Ph	P1	H	H	H	C8H17	H	F	H	H
	213	Ir	3	0	Ph	P1	C8H17	H	H	H	H	H	F	H
	214	Ir	3	0	Ph	P1	H	C8H17	H	H	H	H	F	H
35	215	Ir	3	0	Ph	P1	H	H	C8H17	H	H	H	F	H
	216	Ir	3	0	Ph	P1	H	H	H	C8H17	H	H	F	H
	217	Ir	3	0	Ph	P1	C8H17	H	H	H	H	H	H	F
40	218	Ir	3	0	Ph	P1	H	C8H17	H	H	H	H	H	F
	219	Ir	3	0	Ph	P1	H	H	C8H17	H	H	H	H	F
	220	Ir	3	0	Ph	P1	H	H	H	C8H17	H	H	H	F
45	221	Ir	3	0	Ph	P1	C8H17	H	H	H	CF3	H	H	H
	222	Ir	3	0	Ph	P1	H	C8H17	H	H	CF3	H	H	H
	223	Ir	3	0	Ph	P1	H	H	C8H17	H	CF3	H	H	H
	224	Ir	3	0	Ph	P1	H	H	H	C8H17	CF3	H	H	H
50	225	Ir	3	0	Ph	P1	C8H17	H	H	H	H	CF3	H	H
	226	Ir	3	0	Ph	P1	H	C8H17	H	H	H	CF3	H	H
	227	Ir	3	0	Ph	P1	H	H	C8H17	H	H	CF3	H	H
55	228	Ir	3	0	Ph	P1	H	H	H	C8H17	H	CF3	H	H
	229	Ir	3	0	Ph	P1	C8H17	H	H	H	H	H	CF3	H
	230	Ir	3	0	Ph	P1	H	C8H17	H	H	H	H	CF3	H

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Table 1-4 (continued)

No	M	m	n	A	B	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
231	Ir	3	0	Ph	P1	H	H	C8H17	H	H	H	CF3	H
232	Ir	3	0	Ph	P1	H	H	H	C8H17	H	H	CF3	H
233	Ir	3	0	Ph	P1	C8H17	H	H	H	H	H	H	CF3
234	Ir	3	0	Ph	P1	H	C8H17	H	H	H	H	H	CF3
235	Ir	3	0	Ph	P1	H	H	C8H17	H	H	H	H	CF3
236	Ir	3	0	Ph	P1	H	H	H	C8H17	H	H	H	CF3
237	Ir	3	0	Ph	P1	F	H	H	H	H	H	H	H
238	Ir	3	0	Ph	P1	H	F	H	H	H	H	H	H
239	Ir	3	0	Ph	P1	H	H	F	H	H	H	H	H
240	Ir	3	0	Ph	P1	H	H	H	F	H	H	H	H

Table 1-5

No	M	m	n	A	B	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
241	Ir	3	0	Ph	P1	F	F	H	H	H	H	H	H
242	Ir	3	0	Ph	P1	F	H	F	H	H	H	H	H
243	Ir	3	0	Ph	P1	H	F	H	F	H	H	H	H
244	Ir	3	0	Ph	P1	H	F	F	H	H	H	H	H
245	Ir	3	0	Ph	P1	H	F	H	H	H	H	H	H
246	Ir	3	0	Ph	P1	H	H	H	F	H	H	H	H
247	Ir	3	0	Ph	P1	H	H	F	F	H	H	H	H
248	Ir	3	0	Ph	P1	F	H	F	F	H	H	H	H
249	Ir	3	0	Ph	P1	F	F	F	H	H	H	H	H
250	Ir	3	0	Ph	P1	H	F	F	F	H	H	H	H
251	Ir	3	0	Ph	P1	F	F	F	H	H	H	H	H
252	Ir	3	0	Ph	P1	F	F	F	F	H	H	H	H
253	Ir	3	0	Ph	P1	F	H	H	H	CH3	H	H	H
254	Ir	3	0	Ph	P1	F	H	H	H	H	CH3	H	H
255	Ir	3	0	Ph	P1	F	H	H	H	H	H	CH3	H
256	Ir	3	0	Ph	P1	F	H	H	H	H	H	H	CH3
257	Ir	3	0	Ph	P1	H	F	H	H	CH3	H	H	H
258	Ir	3	0	Ph	P1	H	F	H	H	H	CH3	H	H
259	Ir	3	0	Ph	P1	H	F	H	H	H	H	CH3	H
260	Ir	3	0	Ph	P1	H	F	H	H	H	H	H	CH3
261	Ir	3	0	Ph	P1	H	H	F	H	CH3	H	H	H
262	Ir	3	0	Ph	P1	H	H	F	H	H	CH3	H	H
263	Ir	3	0	Ph	P1	H	H	F	H	H	H	CH3	H
264	Ir	3	0	Ph	P1	H	H	F	H	H	H	H	CH3
265	Ir	3	0	Ph	P1	H	H	H	F	CH3	H	H	H

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Table 1-5 (continued)

No	M	m	n	A	B	A-R1	A-R2	A-R3	A-R4	B-R5	B-R8	B-R7	B-R8
266	Ir	3	0	Ph	P1	H	H	H	F	H	CH3	H	H
267	Ir	3	0	Ph	P1	H	H	H	F	H	H	CH3	H
268	Ir	3	0	Ph	P1	H	H	H	F	H	H	H	CH3
269	Ir	3	0	Ph	P1	F	F	H	H	CH3	H	H	H
270	Ir	3	0	Ph	P1	F	F	H	H	H	CH3	H	H
271	Ir	3	0	Ph	P1	F	F	H	H	H	H	CH3	H
272	Ir	3	0	Ph	P1	F	F	H	H	H	H	H	CH3
273	Ir	3	0	Ph	P1	F	H	F	H	CH3	H	H	H
274	Ir	3	0	Ph	P1	F	H	F	H	H	CH3	H	H
275	Ir	3	0	Ph	P1	F	H	F	H	H	H	CH3	H
276	Ir	3	0	Ph	P1	F	H	F	H	H	H	H	CH3
277	Ir	3	0	Ph	P1	F	H	H	F	CH3	H	H	H
278	Ir	3	0	Ph	P1	F	H	H	F	H	CH3	H	H
279	Ir	3	0	Ph	P1	F	H	H	F	H	H	CH3	H
280	Ir	3	0	Ph	P1	F	H	H	F	H	H	H	CH3
281	Ir	3	0	Ph	P1	H	F	F	H	CH3	H	H	H
282	Ir	3	0	Ph	P1	H	F	F	H	H	CH3	H	H
283	Ir	3	0	Ph	P1	H	F	F	H	H	H	CH3	H
284	Ir	3	0	Ph	P1	H	F	F	H	H	H	H	CH3
285	Ir	3	0	Ph	P1	H	F	H	F	CH3	H	H	H
286	Ir	3	0	Ph	P1	H	F	H	F	H	CH3	H	H
287	Ir	3	0	Ph	P1	H	F	H	F	H	H	CH3	H
288	Ir	3	0	Ph	P1	H	F	H	F	H	H	H	CH3
289	Ir	3	0	Ph	P1	H	H	F	F	CH3	H	H	H
290	Ir	3	0	Ph	P1	H	H	F	F	H	CH3	H	H
291	Ir	3	0	Ph	P1	H	H	F	F	H	H	CH3	H
292	Ir	3	0	Ph	P1	H	H	F	F	H	H	H	CH3
293	Ir	3	0	Ph	P1	F	F	F	H	CH3	H	H	H
294	Ir	3	0	Ph	P1	F	F	F	H	H	CH3	H	H
295	Ir	3	0	Ph	P1	F	F	F	H	H	H	CH3	H
296	Ir	3	0	Ph	P1	F	F	F	H	H	H	H	CH3
291	Ir	3	0	Ph	5P1	F	F	H	F	CH3	H	H	H
298	Ir	3	0	Ph	P1	F	F	H	F	H	CH3	H	H
299	Ir	3	0	Ph	P1	F	F	H	F	H	H	CH3	H
300	Ir	3	0	Ph	P1	F	F	H	F	H	H	H	CH3

Table 1-6

	No	M	m	n	A	B	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
5	301	Ir	3	0	Ph	P1	F	H	F	F	CH3	H	H	H
	302	Ir	3	0	Ph	P1	F	H	F	F	H	CH3	H	H
	303	Ir	3	0	Ph	P1	F	H	F	F	H	H	CH3	H
	304	Ir	3	0	Ph	P1	F	H	F	F	H	H	H	CH3
10	305	Ir	3	0	Ph	P1	F	F	F	F	CH3	H	H	H
	306	Ir	3	0	Ph	P1	F	F	F	F	H	CH3	H	H
	307	Ir	3	0	Ph	P1	F	F	F	F	H	H	CH3	H
15	308	Ir	3	0	Ph	P1	F	F	F	F	H	H	H	CH3
	309	Ir	3	0	Ph	P1	CF3	H	H	H	H	H	H	H
	310	Ir	3	0	Ph	P1	H	CF3	H	H	H	H	H	H
20	311	Ir	3	0	Ph	P1	H	H	CF3	H	H	H	H	H
	312	Ir	3	0	Ph	P1	H	CF3	H	CF3	H	H	H	H
	313	Ir	3	0	Ph	P1	CF3	CF3	H	H	H	H	H	H
	314	Ir	3	0	Ph	P1	CF3	H	CF3	H	H	H	H	H
25	315	Ir	3	0	Ph	P1	CF3	H	H	CF3	H	H	H	H
	316	Ir	3	0	Ph	P1	H	CF3	CF3	H	H	H	H	H
	317	Ir	3	0	Ph	P1	H	H	C3F7C2H4	H	H	H	H	H
30	318	Ir	3	0	Ph	P1	H	H	C7F15	H	H	H	H	H
	316	Ir	3	0	Ph	P1	H	H	CF3	CF3	H	H	H	H
	320	Ir	3	0	Ph	P1	CF3	H	CF3	CF3	H	K	H	H
	321	Ir	3	0	Ph	P1	CF3	CF3	CF3	H	H	H	M	H
35	322	Ir	3	0	Ph	P1	H	CF3	CF3	CF3	H	H	H	H
	323	Ir	3	0	Ph	P1	CF3	CF3	CF3	H	H	H	H	H
	324	Ir	3	0	Ph	P1	CF3	CF3	CF3	CF3	H	H	H	H
40	325	Ir	3	0	Ph	P1	CF3	H	H	H	CH3	H	H	H
	326	Ir	3	0	Ph	P1	CF3	H	H	H	H	CH3	H	H
	327	Ir	3	0	Ph	P1	CF3	H	H	H	H	H	CH3	H
	328	Ir	3	0	Ph	P1	CF3	H	H	H	H	H	H	CH3
45	329	Ir	3	0	Ph	P1	H	CF3	H	H	CH3	H	H	H
	330	Ir	3	0	Ph	P1	H	CF3	H	H	H	CH3	H	H
	331	Ir	3	0	Ph	P1	H	CF3	H	H	H	H	CH3	H
50	332	Ir	3	0	Ph	P1	H	H	H	H	H	H	H	CH3
	333	Ir	3	0	Ph	P1	H	H	CF3	H	CH3	H	H	H
	334	Ir	3	0	Ph	P1	H	H	CF3	H	H	CH3	H	H
	335	Ir	3	0	Ph	P1	H	H	CF3	H	H	H	CH3	H
55	336	Ir	3	0	Ph	P1	H	H	CF3	H	H	H	H	CH3
	337	Ir	3	0	Ph	P1	H	H	H	CF3	CH3	H	H	H

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Table 1-6 (continued)

No	M	m	n	A	B	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
338	Ir	3	0	Ph	P1	H	H	H	CF3	H	CH3	H	H
339	Ir	3	0	Ph	P1	H	H	H	CF3	H	H	CH3	H
340	Ir	3	0	Ph	P1	H	H	H	CF3	H	H	H	CH3
341	Ir	3	0	Ph	P1	CF3	CF3	H	H	CH3	H	H	H
342	Ir	3	0	Ph	P1	CF3	CF3	H	H	H	CH3	H	H
343	Ir	3	0	Ph	P1	CF3	CF3	H	H	H	H	CH3	H
344	Ir	3	0	Ph	P1	CF3	CF3	H	H	H	H	H	CH3
345	Ir	3	0	Ph	P1	CF3	H	CF3	H	CH3	H	H	H
346	Ir	3	0	Ph	P1	CF3	H	CF3	H	H	CH3	H	H
347	Ir	3	0	Ph	P1	CF3	H	CF3	H	H	H	CH3	H
348	Ir	3	0	Ph	P1	CF3	H	CF3	H	H	H	H	CH3
349	Ir	3	0	Ph	P1	CF3	H	H	CF3	CH3	H	H	H
350	Ir	3	0	Ph	P1	CF3	H	H	CF3	H	CH3	H	H
351	Ir	3	0	Ph	P1	CF3	H	H	CF3	H	H	CH3	H
352	Ir	3	0	Ph	P1	CF3	H	H	CF3	H	H	H	CH3
353	Ir	3	0	Ph	P1	H	CF3	CF3	H	CH3	H	H	H
354	Ir	3	0	Ph	P1	H	CF3	CF3	H	H	CH3	H	H
355	Ir	3	0	Ph	P1	H	CF3	CF3	H	H	H	CH3	H
356	Ir	3	0	Ph	P1	H	CF3	CF3	H	H	H	H	CH3
357	Ir	3	0	Ph	P1	H	CF3	H	CF3	CH3	H	H	H
358	Ir	3	0	Ph	P1	H	CF3	H	CF3	H	CH3	H	H
359	Ir	3	0	Ph	P1	H	CF3	H	CF3	H	H	CH3	H
360	Ir	3	0	Ph	P1	H	CF3	H	CF3	H	H	H	CH3

Table 1-7

No	M	m	n	A	B	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
361	Ir	3	0	Ph	P1	H	H	CF3	CF3	CH3	H	H	H
392	Ir	3	0	Ph	P1	H	H	CF3	CF3	H	CH3	H	H
383	Ir	3	0	Ph	P1	H	H	CF3	CF3	H	H	CH3	H
364	Ir	3	0	Ph	P1	H	H	CF3	CF3	H	H	H	CH3
365	Ir	3	0	Ph	P1	CF3	CF3	CF3	H	CH3	H	H	H
368	Ir	3	0	Ph	P1	CF3	CF3	CF3	H	H	CH3	H	H
367	Ir	3	0	Ph	P1	CF3	CF3	CF3	H	H	H	CH3	H
368	Ir	3	0	Ph	P1	CF3	CF3	CF3	H	H	H	H	CH3
369	Ir	3	0	Ph	P1	CF3	CF3	H	CF3	CH3	H	H	H
370	Ir	3	0	Ph	P1	CF3	CF3	H	CF3	H	CH3	H	H
371	Ir	3	0	Ph	P1	CF3	CF3	H	CF3	H	H	CH3	H
372	Ir	3	0	Ph	P1	CF3	CF3	H	CF3	H	H	H	CH3

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Table 1-7 (continued)

No	M	m	n	A	B	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
373	Ir	3	0	Ph	P1	CF3	H	CF3	CF3	CH3	H	H	H
374	Ir	3	0	Ph	P1	CF3	H	CF3	CF3	H	CH3	H	H
375	Ir	3	0	Ph	P1	CF3	H	CF3	CF3	H	H	CH3	H
376	Ir	3	0	Ph	P1	CF3	H	CF3	CF3	H	H	H	CH3
377	Ir	3	0	Ph	P1	CF3	CF3	CF3	CF3	CH3	H	H	H
37B	Ir	3	0	Ph	P1	CF3	CF3	CF3	CF3	H	CH3	H	H
379	Ir	3	0	Ph	P1	CF3	CF3	CF3	CF3	H	H	CH3	H
380	Ir	3	0	Ph	P1	CF3	CF3	CF1	CF3	H	H	H	CH3
381	Ir	3	0	Ph	P1	F	CF3	H	H	H	H	H	H
38Z	Ir	3	0	Ph	P1	F	CF3	H	CF3	H	H	H	H
383	Ir	3	0	Ph	P1	F	H	H	CF3	H	H	H	H
384	Ir	3	0	Ph	P1	H	CF3	F	H	H	H	H	H
385	Ir	3	0	Ph	P1	H	CF3	F	CF3	H	H	H	H
386	Ir	3	0	Ph	P1	H	H	F	CF3	H	H	H	H
387	Ir	3	0	Ph	P1	F	CF3	F	H	H	H	H	H
388	Ir	3	0	Ph	P1	F	H	F	CF3	H	H	H	H
389	Ir	3	0	Ph	P1	H	CH3	F	H	H	H	H	H
390	Ir	3	0	Ph	P1	H	CH3	CF3	H	H	H	H	H
39f	Ir	3	0	Ph	P1	F	CF3	H	CF3	H	H	H	H
392	Ir	3	0	Ph	P1	CF3	H	F	H	H	H	H	H
393	Ir	3	0	Ph	P1	H	CF3	F	H	H	CH3	H	H
394	Ir	3	0	Ph	P1	H	CF3	F	CF3	H	CH3	H	H
395	Ir	3	0	Ph	P1	H	H	F	CF3	H	CH3	H	H
396	Ir	3	0	Ph	P1	F	CF3	F	H	H	CH3	H	H
397	Ir	3	0	Ph	P1	F	H	F	CF3	H	CH3	H	H
398	Ir	3	0	Ph	P1	F	CF3	F	CF3	H	CH3	H	H
399	Ir	3	0	Ph	P1	F	CF3	H	H	H	H	CH3	H
400	Ir	3	0	Ph	P1	F	CF3	H	CF3	H	H	CH3	H
401	Ir	3	0	Ph	P1	F	H	H	CF3	H	H	CH3	H
402	Ir	3	0	Ph	P1	H	CF3	F	H	H	H	CH3	H
403	Ir	3	0	Ph	P1	H	CF3	F	CF3	H	H	CH3	H
404	Ir	3	0	Ph	P1	H	H	F	CF3	H	H	CH3	H
405	Ir	3	0	Ph	P1	F	CF3	F	H	H	H	CH3	H
406	Ir	3	0	Ph	P1	F	H	F	CF3	H	H	CH3	H
407	Ir	3	0	Ph	P1	F	CF3	F	CF3	H	H	CH3	H
406	Ir	3	0	Ph	P1	F	H	H	H	H	CF3	H	H
409	Ir	3	0	Ph	P1	H	F	H	H	H	CF3	H	H
410	Ir	3	0	Ph	P1	H	H	F	H	H	CF3	H	H

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Table 1-7 (continued)

No	M	m	n	A	B	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
411	Ir	3	0	Ph	P1	H	H	H	F	H	CF3	H	H
412	Ir	3	0	Ph	P1	F	H	H	H	H	H	CF3	H
413	Ir	3	0	Ph	P1	H	F	H	H	H	H	CF3	H
414	Ir	3	0	Ph	P1	H	H	F	H	H	H	CF3	H
415	Ir	3	0	Ph	P1	H	H	H	F	H	H	CF3	H
418	Ir	3	0	Ph	P1	H	F	H	F	H	CF3	H	H
417	Ir	3	0	Ph	P1	H	F	H	F	H	CF3	H	H
418	Ir	3	0	Ph	P1	H	F	H	F	H	CF3	H	H
419	Ir	3	0	Ph	P1	H	F	H	F	H	CF3	H	H
420	Ir	3	0	Ph	P1	H	F	H	F	H	H	CF3	H

Table 1-8

No	M	m	n	A	B	E	J	G	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
421	Ir	3	0	Ph	P1	-	-	-	H	F	H	F	H	H	CF3	H
422	Ir	3	0	Ph	P1	-	-	-	H	F	H	F	H	H	CF3	H
423	Ir	3	0	Ph	P1	-	-	-	H	F	H	F	H	H	CF3	H
424	Ir	3	0	Ph	P1	-	-	-	CF3	H	H	H	H	CF3	H	H
425	Ir	3	0	Ph	P1	-	-	-	H	CF3	H	H	H	CF3	H	H
426	Ir	3	0	Ph	P1	-	-	-	H	H	CF3	H	H	CF3	H	H
427	Ir	3	0	Ph	P1	-	-	-	H	H	H	CF3	H	CF3	H	H
428	Ir	3	0	Ph	P1	-	-	-	CF3	H	H	H	H	H	CF3	H
429	Ir	3	0	Ph	P1	-	-	-	H	CF3	H	H	H	H	CF3	H
430	Ir	3	0	Ph	P1	-	-	-	H	H	CF3	H	H	H	CF3	H
431	Ir	3	0	Ph	P1	-	-	-	H	H	H	CF3	H	H	CF3	H
432	Ir	3	0	Ph	P1	-	-	-	CF3	H	CF3	H	H	CF3	H	H
433	Ir	3	0	Ph	P1	-	-	-	H	F	CF3	H	H	CF3	H	H
434	Ir	3	0	Ph	P1	-	-	-	CF3	H	CF3	H	H	CF3	H	H
435	Ir	3	0	Ph	P1	-	-	-	H	H	H	CF3	H	CF3	H	H
436	Ir	3	0	Ph	P1	-	-	-	CF3	H	CF3	H	H	H	CF3	H
437	Ir	3	0	Ph	P1	-	-	-	H	F	CF3	H	H	H	CF3	H
438	Ir	3	0	Ph	P1	-	-	-	CF3	H	CF3	H	H	H	CF3	H
439	Ir	3	0	Ph	P1	-	-	-	H	H	H	CF3	H	H	CF3	H
440	Ir	2	1	Ph	P1	CH3	H	CH3	CH3	H	H	H	H	H	H	H
441	Ir	2	1	Ph	P1	CH3	H	CH3	H	CH3	H	H	H	H	H	H
442	Ir	2	1	Ph	P1	CH3	H	CH3	H	H	CH3	H	H	H	H	H
443	Ir	2	1	Ph	P1	CH3	H	CH3	H	H	H	CH3	H	H	H	H
444	Ir	2	1	Ph	P1	CH3	H	CH3	C2H5	H	H	H	H	H	H	H
445	Ir	2	1	Ph	P1	CH3	H	CH3	H	C2H5	H	H	H	H	H	H

Table 1-8 (continued)

No	M	m	n	A	B	E	J	G	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
446	Ir	2	1	Ph	P1	CH3	H	CH3	H	H	C2H5	H	H	H	H	H
447	Ir	2	1	Ph	P1	CH3	H	CH3	H	H	H	C2H5	H	H	H	H
448	Ir	2	1	Ph	P1	CH3	H	CH3	C3H7	H	H	H	H	H	H	H
449	Ir	2	1	Ph	P1	CH3	H	CH3	H	C3H7	H	H	H	H	H	H
450	Ir	2	1	Ph	P1	CH3	H	CH3	H	H	C3H7	H	H	H	H	H
451	Ir	2	1	Ph	P1	CH3	H	CH3	H	H	H	C3H7	H	H	H	H
452	Ir	2		1 Ph	Pt	CH3	H	CH3	C4H9	H	H	H	H	H	H	H
453	Ir	2	1	Ph	P1	CH3	H	CH3	H	C4H9	H	H	H	H	H	H
454	Ir	2	1	Ph	P1	CH3	H	CH3	H	H	C4H9	H	H	H	H	H
455	Ir	2	1	Ph	P1	CH3	H	CH3	H	H	H	C4H9	H	H	H	H
456	Ir	2	1	Ph	P1	CH3	H	CH3	C6H13	H	H	H	H	H	H	H
457	Ir	2	1	Ph	P1	CH3	H	CH3	H	C6H13	H	H	H	H	H	H
458	Ir	2	1	Ph	P1	CH3	H	CH3	H	H	C6H13	H	H	H	H	H
459	Ir	2	1	Ph	P1	CH3	H	CH3	H	H	H	C6H13	H	H	H	H
460	Ir	2	1	Ph	P1	CH3	H	CH3	C8H17	H	H	H	H	H	H	H
461	Ir	2	1	Ph	P1	CH3	H	CH3	H	C8H17	H	H	H	H	H	H
462	Ir	2	1	Ph	P1	CH3	H	CH3	H	H	C8H17	H	H	H	H	H
463	Ir	2	1	Ph	P1	CH3	H	CH3	H	H	H	C8H17	H	H	H	H
464	Ir	2	1	Ph	P1	CH3	H	CH3	C12H25	H	H	H	H	H	H	H
465	Ir	2	1	Ph	P1	CH3	H	CH3	H	C12H25	H	H	H	H	H	H
466	Ir	2	1	Ph	P1	CH3	H	CH3	H	H	C12H25	H	H	H	H	H
467	Ir	2	1	Ph	P1	CH3	H	CH3	H	H	H	C12H25	H	H	H	H
468	Ir	2	1	Ph	P1	CH3	H	CH3	C15H31	H	H	H	H	H	H	H
469	Ir	2	1	Ph	P1	CH3	H	CH3	H	C15H31	H	H	H	H	H	H
470	Ir	2	1	Ph	P1	CH3	H	CH3	H	H	C15H31	H	H	H	H	H

Table 1-8 (continued)

No	M	m	n	A	B	E	J	G	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
471	Ir	2	1	Ph	P1	CH3	H	CH3	H	H	H	C15H31	H	H	H	H
472	Ir	2	1	Ph	Pt	CH3	CH3	CH3	H	H	H	H	H	H	H	H
473	Ir	2	1	Ph	P1	CH3	F	CH3	H	H	H	H	H	H	H	H
474	Ir	2	1	Ph	P1	CF3	CH3	CF3	H	H	H	H	H	H	H	H
475	Ir	2	1	Ph	P1	CF3	F	CF3	H	H	H	H	H	H	H	H
476	Ir	2	1	Ph	P1	CH3	CF3	CH3	H	H	H	H	H	H	H	H
477	Ir	2	1	Ph	P1	C4H9	F	C4H9	H	H	H	H	H	H	H	H
478	Ir	2	1	Ph	P1	CH3	C2HS	CH3	H	H	H	H	H	H	H	H
479	Ir	2	1	Ph	P1	CH3	C4H9	CH3	H	H	H	H	H	H	H	H
480	Ir	2	1	Ph	P1	CH3	CH3	CH3	H	CH3	H	H	H	H	H	H

Table 1-9

No	M	m	n	A	B	E	J	G	A-A1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
481	Ir	2	1	Ph	P1	CH3	F	CH3	H	CH3	H	H	H	H	H	H
482	Ir	2	1	Ph	P1	CF3	CH3	CF3	H	CH3	H	H	H	H	H	H
483	Ir	2	1	Ph	P1	CF3	F	CF3	H	CH3	H	H	H	H	H	H
484	Ir	2	1	Ph	P1	CH3	CF3	CH3	H	CH3	H	H	H	H	H	H
485	Ir	2	1	Ph	P1	C4H9	F	C4H9	H	CH3	H	H	H	H	H	H
488	Ir	2	1	Ph	P1	CH3	C2H5	CH3	H	CH3	H	H	H	H	H	H
487	Ir	2	1	Ph	P1	CH3	H	CH3	H	F	H	H	H	H	H	H
488	Ir	2	1	Ph	P1	CH3	CH3	CH3	H	F	H	H	H	H	H	H
489	Ir	2	1	Ph	P1	CH3	H	CH3	H	H	F	H	H	H	H	H
490	Ir	2	1	Ph	P1	CF3	CH3	CF3	H	F	H	H	H	H	H	H
491	Ir	2	1	Ph	P1	CF3	F	CF3	H	F	H	H	H	H	H	H
492	Ir	2	1	Ph	P1	CH3	CF3	CH3	H	F	H	H	H	H	H	H
493	Ir	2	1	Ph	P1	C4H9	F	C4H9	H	F	H	H	H	H	H	H
494	Ir	2	1	Ph	P1	CH3	C2H5	CH3	H	F	H	H	H	H	H	H
495	Ir	2	1	Ph	P1	CH3	H	CH3	H	CF3	H	H	H	H	H	H
496	Ir	2	1	Ph	P1	CH3	CH3	CH3	H	CF3	H	H	H	H	H	H
497	Ir	2	1	Ph	P1	CH3	F	CH3	H	CF3	H	H	H	H	H	H
498	Ir	2	1	Ph	P1	CF3	CH3	CF3	H	CF3	H	H	H	H	H	H
499	Ir	2	1	Ph	P1	CF3	F	CF3	H	CF3	H	H	H	H	H	H
500	Ir	2	1	Ph	P1	CH3	CF3	CH3	H	CF3	H	H	H	H	H	H
501	Ir	2	1	Ph	P1	C4H9	F	C4H9	H	CF3	H	H	H	H	H	H
502	Ir	2	1	Ph	P1	CH3	C2H5	CH3	H	CF3	H	H	H	H	H	H
503	Ir	2	1	Ph	P1	CH3	H	CH3	H	H	H	H	H	CH3	H	H
504	Ir	2	1	Ph	P1	CH3	CH3	CH3	H	H	H	H	H	CH3	H	H
505	Ir	2	1	Ph	P1	CH3	F	CH3	H	H	H	H	H	CH3	H	H

Table 1-9 (continued)

No	M	m	n	A	B	E	J	G	A-A1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
506	Ir	2	1	Ph	P1	CF3	CH3	CF3	H	H	H	H	H	CH3	H	H
507	Ir	2	1	Ph	P1	CF3	F	CF3	H	H	H	H	H	CH3	H	H
508	Ir	2	1	Ph	P1	CH3	CF3	CH3	H	H	H	H	H	CH3	H	H
509	Ir	2	1	Ph	P1	C4H9	F	C4H9	H	H	H	H	H	CH3	H	H
510	Ir	2	1	Ph	P1	CH3	C2H5	CH3	H	H	H	H	H	CH3	H	H
511	Ir	2	1	Ph	P1	CH3	H	CH3	H	H	H	H	H	H	CH3	H
512	Ir	2	1	Ph	P1	CH3	CH3	CH3	H	H	H	H	H	H	CH3	H
513	Ir	2	1	Ph	P1	CH3	F	CH3	H	H	H	H	H	H	CH3	H
514	Ir	2	1	Ph	P1	CF3	CH3	CF3	H	H	H	H	H	H	CH3	H
515	Ir	2	1	Ph	P1	CF3	F	CF3	H	H	H	H	H	H	CH3	H
516	Ir	2	1	Ph	P1	CH3	CF3	CH3	H	H	H	H	H	H	CH3	H
517	Ir	2	1	Ph	P1	C4H9	F	C4H9	H	H	H	H	H	H	CH3	H
518	Ir	2	1	Ph	P1	CH3	C2H5	CH3	H	H	H	H	H	H	CH3	H
819	Ir	2	1	Ph	P1	CH3	H	CH3	H	CF3	F	H	H	CH3	H	H
520	Ir	2	1	Ph	P1	CH3	CH3	CH3	H	CF3	F	H	H	CH3	H	H
521	Ir	2	1	Ph	P1	CH3	F	CH3	H	CF3	F	H	H	CH3	H	H
522	Ir	2	1	Ph	P1	CF3	CH3	CF3	H	CF3	F	H	H	CH3	H	H
523	Ir	2	1	Ph	P1	CF3	F	CF3	H	CF3	F	H	H	CH3	H	H
524	Ir	2	1	Ph	P1	CH3	CF3	CH3	H	CF3	F	H	H	CH3	H	H
525	Ir	2	1	Ph	P1	C4H9	F	C4H9	H	CF3	F	H	H	CH3	H	H
528	Ir	2	1	Ph	P1	CH3	C2H5	CH3	H	CF3	F	H	H	CH3	H	H
527	Ir	2	1	Ph	P1	CH3	H	CH3	F	H	F	H	H	H	CH3	H
528	Ir	2	1	Ph	P1	CH3	CH3	CH3	F	H	F	H	H	H	CH3	H
529	Ir	2	1	Ph	P1	CH3	F	CH3	F	H	F	H	H	H	CH3	H
530	Ir	2	1	Ph	P1	CF3	CH3	CF3	F	H	F	H	H	CH3	H	H

Table 1-9 (continued)

No	M	m	n	A	B	E	J	G	A-A1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
531	Ir	2	1	Ph	P1	CF3	F	CF3	F	H	F	H	H	H	CH3	H
532	Ir	2	1	Ph	P1	CH3	CF3	CH3	F	H	F	H	H	H	CH3	H
533	Ir	2	1	Ph	P1	C4H9	F	C4H9	F	H	F	H	H	H	CH3	H
534	Ir	2	1	Ph	P1	CH3	C2H5	CH3	F	H	F	H	H	H	CH3	H
535	Ir	2	1	Ph	P1	CH3	H	CH3	H	F	H	F	H	H	H	H
536	Ir	2	1	Ph	P1	CH3	CH3	CH3	H	F	H	F	H	H	H	H
537	Ir	2	1	Ph	P1	CH3	F	CH3	H	F	H	F	H	H	H	H
538	Ir	2	1	Ph	P1	CF3	CH3	CF3	H	F	M	F	H	H	CH3	H
539	Ir	2	1	Ph	P1	CF3	F	CF3	H	H	F	H	H	H	CF3	H
540	Ir	2	1	Ph	P1	CH3	CF3	CH3	H	H	F	H	H	H	CF3	H

Table 1-10

No	M	m	n	A	B	B'orB	E	J	C	A-R1	A-R2	A-R3	A-R4	B-R5	B-R8	B-R7	B-R8
541	Ir	2	1	Ph	P1	-	C4H9	F	C4H9	H	H	F	H	H	H	CF3	H
542	Ir	2	1 Ph		P1	-	CH3	C2H5	CH3	H	H	F	H	H	H	CF3	H
543	Ir	2	1	Ph	P1	-	CH3	H	CH3	H	H	F	H	H	CF3	H	H
544	Ir	2	1	Ph	P1	-	CH3	CH3	CH3	H	H	F	H	H	CF3	H	H
545	Ir	2	1	Ph	P1	-	CH3	F	CH3	H	H	F	H	H	CP3	H	H
546	Ir	2	1	Ph	P1	-	CF3	CH3	CF3	H	H	F	H	H	CF3	H	H
547	Ir	2	1	Ph	P1	-	CF3	F	CF3	H	H	F	H	H	CF3	H	H
548	Ir	2	1	Ph	P1	-	CH3	CF3	CH3	H	H	F	H	H	CF3	H	H
549	Ir	2	1	Ph	P1	-	C4H9	F	C4H9	H	H	F	H	H	CF3	H	H
550	Ir	2	1	Ph	P1	-	CH3	C2H5	CH3	H	H	F	H	H	CF3	H	H
551	Ir	2	1	Ph	P1	-	CH3	H	CH3	H	CF3	F	H	H	H	H	H
552	Ir	2	1	Ph	P1	-	CH3	CH3	CH3	H	CF3	F	H	H	H	H	H
553	Ir	2	1	Ph	P1	-	CH3	F	CH3	H	CF3	F	H	H	H	H	H
554	Ir	2	1	Ph	P1	-	CF3	CH3	CF3	H	CP3	F	H	H	H	H	H
555	Ir	2	1	Ph	P1	-	CF3	F	CF3	H	CF3	F	H	H	H	H	H
556	Ir	2	1	Ph	P1	-	CH3	CF3	CH3	H	CF3	F	H	H	H	H	H
557	Ir	2	1	Ph	P1	-	C4H9	F	C4H9	H	CF3	F	H	H	H	H	H
558	Ir	2	1	Ph	P1	-	CH3	C2H5	CH3	H	CP3	F	H	H	H	H	H
559	Ir	2	1	Ph	P1	-	CH3	H	CH3	H	CF3	F	H	H	H	CH3	H
560	Ir	2	1	Ph	P1	-	CH3	CH3	CH3	H	CF3	F	H	H	H	CH3	H
561	Ir	2	1	Ph	P1	-	CH3	F	CH3	H	CF3	F	H	H	H	CH3	H
562	Ir	2	1	Ph	P1	-	CF3	CH3	CP3	H	CF3	F	H	H	H	CH3	H
563	Ir	2	1	Ph	P1	-	CF3	F	CF3	H	CF3	F	H	H	H	CH3	H
564	Ir	2	1	Ph	P1	-	CH3	CF3	CH3	H	CF3	F	H	H	H	CH3	H
565	Ir	2	1	Ph	P1	-	C4H9	F	C4H9	H	CF3	F	H	H	H	CH3	H

Table 1-10 (continued)

No	M	m	n	A	B	B or B	E	J	C	A-R1	A-R2	A-R3	A-R4	B-R5	B-R8	B-R7	B-R8
566	Ir	2	1	Ph	P1	-	CH3	C2H5	CH3	H	CF3	F	H	H	H	CH3	H
567	Ir	2	1	Ph	P1	-	CH3	H	CH3	H	CF3	H	CF3	H	H	H	H
568	Ir	2	1	Ph	P1	-	CH3	CH3	CH3	H	CF3	H	CF3	H	H	H	H
569	Ir	2	1	Ph	P1	-	CH3	F	CH3	H	CF3	H	CF3	H	H	H	H
570	Ir	2	1	Ph	P1	-	CF3	CH3	CF3	H	CF3	H	CF3	H	H	H	H
571	Ir	2	1	Ph	P1	-	CF3	F	CF3	H	CF3	H	CF3	H	H	H	H
572	Ir	2	1	Ph	P1	-	CH3	CF3	CH3	H	CF3	H	CF3	H	H	H	H
573	Ir	2	1	Ph	P1	-	C4H9	F	C4H9	H	CF3	H	CF3	H	H	H	H
574	Ir	2	1	Ph	P1	-	CH3	C2H5	CH3	H	CF3	H	H	H	H	H	H
575	Ir	2	1	Ph	P1	P1	-	-	-	H	H	H	H	H	H	C4H9	H
576	Ir	2	1	Ph	P1	P1	-	-	-	F	H	H	H	H	H	C4H9	H
577	Ir	2	1	Ph	P1	P1	-	-	-	H	F	H	H	H	H	C4H9	H
578	Ir	2	1	Ph	P1	P1	-	-	-	H	H	F	H	H	H	C4H9	H
579	Ir	2	1	Ph	P1	P1	-	-	-	H	H	H	F	H	H	C4H9	H
580	Ir	2	1	Ph	P1	P1	-	-	-	F	H	F	H	H	H	C4H9	H
581	Ir	2	1	Ph	P1	P1	-	-	-	H	F	H	F	H	H	C4H9	H
582	Ir	2	1	Ph	P1	P1	-	-	-	H	F	F	H	H	H	C4H9	H
583	Ir	2	1	Ph	P1	P1	-	-	-	F	H	H	F	H	H	C4H9	H
584	Ir	2	1	Ph	P1	P1	-	-	-	F	F	F	F	H	H	C4H9	H
585	Ir	2	1	Ph	P1	P1	-	-	-	H	CF3	H	H	H	H	C4H9	H
586	Ir	2	1	Ph	P1	P1	-	-	-	H	H	H	CF3	H	H	C4H9	H
587	Ir	2	1	Ph	P1	P1	-	-	-	H	CF3	H	CF3	H	H	C4H9	H
588	Ir	2	1	Ph	P1	P1	-	-	-	H	CF3	F	H	H	H	C4H9	H
589	Ir	2	1	Ph	P1	P1	-	-	-	F	CF3	F	H	H	H	C4H9	H
590	Ir	2	1	Ph	P1	P1	-	-	-	F	CF3	H	H	H	H	C4H9	H

Table 1-10 (continued)

No	M	m	n	A	B	B'orB	E	J	C	A-R1	A-R2	A-R3	A-R4	B-R5	B-R7	B-R8
591	Ir	2	1	Ph	P1	P1	-	-	-	H	H	F	CF3	H	C4H9	H
592	Ir	2	1	Ph	P1	P1	-	-	-	F	H	H	CF3	H	C4H9	H
593	Ir	2	1	Ph	P1	P1	-	-	-	F	H	F	CF3	H	C4H9	H
594	Ir	2	1	Ph	P1	P1	-	-	-	H	CH3	H	H	H	C4H9	H
595	Ir	2	1	Ph	P1	P1	-	-	-	H	H	CH3	H	H	C4H9	H
596	Ir	2	1	Ph	P1	P1	-	-	-	H	C2H5	H	H	H	C4H9	H
597	Ir	2	1	Ph	P1	P1	-	-	-	H	H	C2H5	H	H	C4H9	H
598	Ir	2	1	Ph	P1	P1	-	-	-	H	C4H9	H	H	H	C4H9	H
599	Ir	2	1	Ph	P1	P1	-	-	-	H	H	C4H9	H	H	C4H9	H
600	Ir	2	1	Ph	P1	P1	-	-	-	F	H	H	H	H	H	H

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Table 1-11

	No	M	m	n	A	8	B'orB"	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
5	601	Ir	2	1	Ph	P1	P1	H	F	H	H	H	H	H	H
	602	Ir	2	1	Ph	P1	P1	H	H	F	H	H	H	H	H
	603	Ir	2	1	Ph	P1	P1	H	H	H	F	H	H	H	H
	604	Ir	2	1	Ph	P1	P1	H	F	H	F	H	H	H	H
10	605	Ir	2	1	Ph	P1	P1	H	F	F	H	H	H	HH	
	606	Ir	2	1	Ph	P1	P1	F	H	H	F	H	H	H	H
	607	Ir	2	1	Ph	P1	P1	F	F	F	F	H	H	H	H
15	608	Ir	2	1	Ph	P1	P1	H	CF3	H	H	H	H	H	H
	609	Ir	2	1	Ph	P1	P1	H	H	H	CF3	H	H	H	H
	610	Ir	2	1	Ph	P1	P1	H	CF3	H	CF3	H	H	H	H
20	611	Ir	2	1	Ph	P1	P1	H	CF3	F	H	H	H	H	H
	612	Ir	2	1	Ph	P1	P1	F	CF3	F	H	H	H	H	H
	613	Ir	2	1	Ph	P1	P1	F	CF3	H	H	H	H	H	H
	614	Ir	2	1	Ph	P1	P1	H	H	F	CF3	H	H	H	H
25	615	Ir	2	1	Ph	P1	P1	F	H	H	CF3	H	H	H	H
	616	Ir	2	1	Ph	P1	P1	F	H	F	CF3	H	H	H	H
	617	Ir	2	1	Ph	P1	P1	H	CH3	H	H	H	H	H	H
30	616	Ir	2	1	Ph	P1	P1	H	H	CH3	H	H	H	H	H
	619	Ir	2	1	Ph	P1	P1	H	C2H5	H	H	H	H	H	H
	620	Ir	2	1	Ph	P1	P1	H	H	C2H5	H	H	H	H	H
	621	Ir	2	1	Ph	P1	P1	H	C4H9	H	H	H	H	H	H
35	622	Ir	2	1	Ph	Pt	P1	H	H	C4H9	H	H	H	H	H
	623	Ir	2	1	Ph	P1	P1	H	H	H	H	H	H	H	CH3
	624	Ir	2	1	Ph	P1	P1	F	H	H	H	H	H	H	CH3
40	625	Ir	2	1	Ph	P1	P1	H	F	H	H	H	H	H	CH3
	626	Ir	2	1	Ph	P1	P1	H	H	F	H	H	H	H	CH3
	627	Ir	2	1	Ph	P1	P1	H	H	H	F	H	H	H	CH3
	628	Ir	2	1	Ph	P1	P1	F	H	F	H	H	H	H	CH3
45	629	Ir	2	1	Ph	P1	P1	H	F	H	F	H	H	H	CH3
	630	Ir	2	1	Ph	P1	P1	H	F	F	H	H	H	H	CH3
	631	Ir	2	1	Ph	P1	P1	F	H	H	F	H	H	H	CM3
50	632	Ir	2	1	Ph	P1	P1	F	F	F	F	H	H	H	CH3
	633	Ir	2	1	Ph	P1	P1	H	CF3	H	H	H	H	H	CH3
	634	Ir	2	1	Ph	P1	P1	H	H	H	CF3	H	H	H	CH3
	635	Ir	2	1	Ph	P1	P1	H	CF3	H	CF3	H	H	H	CH3
55	636	Ir	2	1	Ph	P1	P1	H	CF3	F	H	H	H	H	CH3
	637	Ir	2	1	Ph	P1	P1	F	CF3	F	H	H	H	H	CH3

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Table 1-11 (continued)

No	M	m	n	A	8	B'orB"	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
5 638	Ir	2	1	Ph	P1	P1	F	CF3	H	H	H	H	H	CH3
639	Ir	2	1	Ph	P1	P1	H	H	F	CF3	H	H	H	CH3
640	Ir	2	1	Ph	P1	P1	F	H	H	CF3	H	H	H	CH3
641	Ir	2	1	Ph	P1	P1	F	H	F	CF3	H	H	H	CH3
10 642	Ir	2	1	Ph	P1	P1	H	CH3	H	H	H	H	H	CH3
643	Ir	2	1	Ph	P1	P1	H	H	CH3	H	H	H	H	CH3
644	Ir	2	1	Ph	P1	P1	H	C2H5	H	H	H	H	H	CH3
645	Ir	2	1	Ph	P1	P1	H	H	C2HS	H	H	H	H	CH3
15 646	Ir	2	1	Ph	P1	P1	H	C4H9	H	H	H	H	H	CH3
647	Ir	2	1	Ph	P1	P1	H	H	C4H9	H	H	H	H	CH3
648	Ir	3	0	Ph	P2	-	H	H	CH3	H	H	H	H	-
20 649	Ir	3	0	Ph	P2	-	H	H	C4H9	H	H	H	H	-
650	Ir	3	0	Ph	P2	-	F	H	F	H	H	H	H	-
651	Ir	3	0	Ph	P2	-	H	H	F	H	H	H	H	-
25 652	Ir	3	0	Ph	P2	-	H	CF3	H	H	H	H	H	-
653	Ir	3	0	Ph	P2	-	H	H	H	H	H	H	H	-
654	Ir	3	0	Ph	P2	-	H	H	H	H	H	H	H	-
655	Ir	3	0	Ph	P2	-	H	H	H	H	H	H	H	-
30 656	Ir	3	0	Ph	P2	-	H	H	H	H	H	H	CH3	-
657	Ir	3	0	Ph	P2	-	H	H	H	H	H	CH3	H	-
658	Ir	3	0	Ph	P3	-	H	H	CH3	H	H	H	H	-
35 659	Ir	3	0	Ph	P3	-	H	H	C4H9	H	H	H	H	-
660	Ir	3	0	Ph	P3	-	F	H	F	H	H	H	H	-

Table 1-12

No	M	m	n	A	B	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
40 661	Ir	3	0	Ph	P3	H	H	F	H	H	H	H	H
662	Ir	3	0	Ph	P3	H	CF3	H	H	H	H	H	-
45 663	Ir	3	0	Ph	P3	H	H	H	H	H	H	H	-
664	Ir	3	0	Ph	P3	H	H	H	H	H	H	H	-
665	Ir	3	0	Ph	P3	H	H	H	H	H	H	H	-
666	Ir	3	0	Ph	P3	H	H	H	H	CH3	H	H	-
50 667	Ir	3	0	Ph	P3	H	H	H	H	H	CH3	H	-
668	Ir	3	0	Ph	P4	H	H	CH3	H	H	H	H	-
669	Ir	3	0	Ph	P4	H	H	C4H9	H	H	H	H	-
55 670	Ir	3	0	Ph	P4	F	H	F	H	H	H	H	-
671	Ir	3	0	Ph	P4	H	H	F	H	H	H	H	-
672	Ir	3	0	Ph	P4	H	CF3	H	H	H	H	H	-

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Table 1-12 (continued)

No	M	m	n	A	B	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
673	Ir	3	0	Ph	P4	H	H	H	H	H	H	H	-
674	Ir	3	0	Ph	P4	H	H	H	H	H	H	H	-
675	Ir	3	0	Ph	P4	H	H	H	H	H	H	H	-
676	Ir	3	0	Ph	P4	H	H	H	H	CH3	H	H	-
677	Ir	3	0	Ph	P4	H	H	H	H	H	CH3	H	-
678	Ir	3	0	Ph	P5	H	CH3	H	H	H	CH3	H	-
679	Ir	3	0	Ph	P5	H	H	C4H9	H	H	H	H	-
680	Ir	3	0	Ph	P5	H	H	F	H	H	H	H	-
681	Ir	3	0	Ph	P5	H	CF3	H	H	H	H	H	-
682	Ir	3	0	Ph	P5	H	H	H	H	H	CH3	H	-
683	Ir	3	0	Ph	P6	H	H	CH3	H	H	H	H	H
684	Ir	3	0	Ph	P6	H	H	C4H9	H	H	H	H	H
685	Ir	3	0	Ph	P6	H	H	F	H	H	H	H	H
686	Ir	3	0	Ph	P6	H	CF3	H	H	H	H	H	H
687	Ir	3	0	Ph	P6	H	H	H	H	H	CH3	H	H
688	Ir	3	0	Ph	P7	H	H	CH3	H	H	H	H	H
689	Ir	3	0	Ph	P7	H	H	C4H9	H	H	H	H	H
690	Ir	3	0	Ph	P7	H	H	F	H	H	H	H	H
691	Ir	3	0	Ph	P7	H	CF3	H	H	H	H	H	H
692	Ir	3	0	Ph	P7	H	H	H	H	H	CH3	H	H
693	Ir	3	0	Ph	P8	H	H	CH3	H	H	H	H	H
694	Ir	3	0	Ph	P8	H	H	C4H9	H	H	H	H	H
695	Ir	3	0	Ph	P8	H	H	F	H	H	H	H	H
696	Ir	3	0	Ph	P9	H	H	H	H	H	H	CH3	H
697	Ir	3	0	Ph	P8	H	H	H	H	H	CH3	H	H
698	Ir	3	0	Ph	P9	H	H	CH3	H	H	H	H	H
699	Ir	3	0	Ph	P9	H	H	C4H9	H	H	H	H	H
700	Ir	3	0	Ph	P9	H	H	F	H	H	H	H	H
701	Ir	3	0	Ph	P9	H	H	H	H	H	H	CH3	H
702	Ir	3	0	Ph	P9	H	H	H	H	H	CH3	H	H

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Table 1-13

Table 1-14

No	M	n	a	A	B	B ^{ext}	E	J	Q	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8	B-R9	B-R10	B-R11	B-R12	B-R13	B-R14	B-R15	B-R16	B-R17	B-R18
744	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
745	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
746	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
747	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
748	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
749	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
750	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
751	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
752	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
753	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
754	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
755	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
756	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
757	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
758	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
759	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
760	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
761	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
762	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
763	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
764	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
765	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
766	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
767	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
768	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
769	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
770	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
771	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
772	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
773	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
774	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
775	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
776	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
777	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
778	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
779	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H
780	F	3	0	Ta3	P1	-	-	-	-	H	H	H	H	H	H	CH3	H	H	H	H	H	H	H	H	H	H	H

Table 1-15

No	M	m	n	q	A	B	8 or 8'	E	J	Q	A-81	A-82	A-83	A-84	B-85	B-86	B-87	B-88	B-89	B-90	B-91	B-92
781	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
782	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
783	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
784	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
785	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
786	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
787	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
788	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
789	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
790	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
791	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
792	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
793	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
794	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
795	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
796	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
797	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
798	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
799	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
800	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
801	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
802	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
803	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
804	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
805	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
806	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
807	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
808	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
809	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
810	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
811	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
812	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
813	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
814	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
815	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
816	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
817	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
818	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
819	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-
820	1	3	0	0	P1	P1	-	-	-	-	H	H	CH3	H	H	H	H	H	H	-	-	-

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Table 1-17

No	M	E	G	A	B	A'	B' or B"	E	J	Q	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8	B'-R5	B'-R6	B'-R7	B'-R8
861	Pt	2	0	Pt	Pt	-	-	-	-	-	H	C2H4O	H	H	H	H	CH3	H	-	-	-	-
862	Pt	2	0	Pt	Pt	-	-	-	-	-	H	CF3	H	H	H	H	CH3	H	-	-	-	-
863	Pt	2	0	Pt	Pt	-	-	-	-	-	H	H	F	H	H	H	CH3	H	-	-	-	-
864	Pt	2	0	Pt	Pt	-	-	-	-	-	H	CF3	F	H	H	H	CH3	H	-	-	-	-
865	Pt	2	0	Pt	Pt	-	-	-	-	-	H	CF3	H	CF3	H	H	CH3	H	-	-	-	-
866	Pt	2	0	Pt	Pt	-	-	-	-	-	F	H	F	H	H	H	CH3	H	-	-	-	-
867	Pt	2	0	Pt	Pt	-	-	-	-	-	F	CF3	F	H	H	H	CH3	H	-	-	-	-
868	Pt	2	0	Pt	Pt	-	-	-	-	-	H	CF3	F	CF3	H	H	CH3	H	-	-	-	-
869	Pt	1	1	Pt	Pt	-	-	-	-	-	H	CH3	H	H	H	H	H	H	-	-	-	-
870	Pt	1	1	Pt	Pt	-	-	-	-	-	H	CH3	F	H	H	H	H	H	-	-	-	-
871	Pt	1	1	Pt	Pt	-	-	-	-	-	H	CH3	F	H	H	H	H	H	-	-	-	-
872	Pt	1	1	Pt	Pt	-	-	-	-	-	H	CF3	F	H	H	H	H	H	-	-	-	-
873	Pt	1	1	Pt	Pt	-	-	-	-	-	H	CF3	F	H	H	H	H	H	-	-	-	-
874	Pt	1	1	Pt	Pt	-	-	-	-	-	H	CF3	F	H	H	H	H	H	-	-	-	-
875	Pt	1	1	Pt	Pt	-	-	-	-	-	H	CF3	F	H	H	H	H	H	-	-	-	-
876	Pt	1	1	Pt	Pt	-	-	-	-	-	CH3	H	H	H	H	H	H	H	-	-	-	-
877	Pd	2	0	Pt	Pt	-	-	-	-	-	H	H	CH3	H	H	H	H	H	-	-	-	-
878	Pd	2	0	Pt	Pt	-	-	-	-	-	H	H	CH3	H	H	H	H	H	-	-	-	-
879	Pd	2	0	Pt	Pt	-	-	-	-	-	H	H	F	H	H	H	H	H	-	-	-	-
880	Pd	2	0	Pt	Pt	-	-	-	-	-	H	CF3	F	H	H	H	H	H	-	-	-	-
881	Pd	2	0	Cs	Pt	-	-	-	-	-	H	CH3	H	H	H	H	H	H	-	-	-	-
882	Pd	1	1	Pt	Pt	-	-	-	-	-	H	H	H	H	H	H	H	H	-	-	-	-
883	Pd	1	1	Pt	Pt	-	-	-	-	-	H	H	CH3	H	H	H	H	H	-	-	-	-

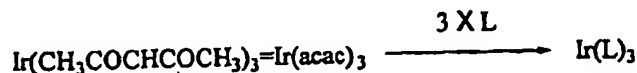
[0061] Hereinbelow, the present invention will be described more specifically based on Examples.

[0062] Iridium metal coordination compounds used in Examples were synthesized along synthesis paths shown below. (Analogous reactions are described in Inorg. Chem. 1994, 33, p. 545).

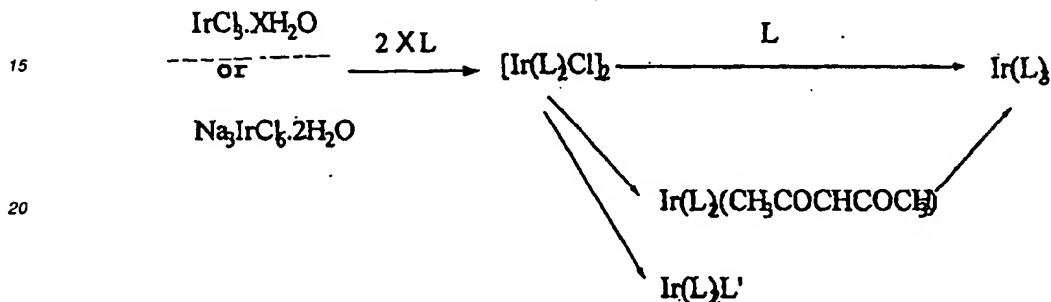
<<Synthesis of iridium metal coordination compounds>>

[0063] A process scheme for synthesizing Iridium complexes used in the present invention is shown below.

5



10 or

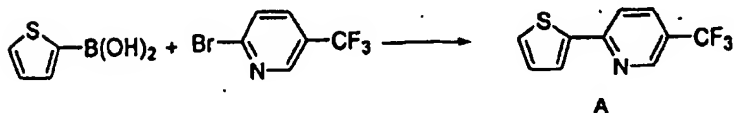


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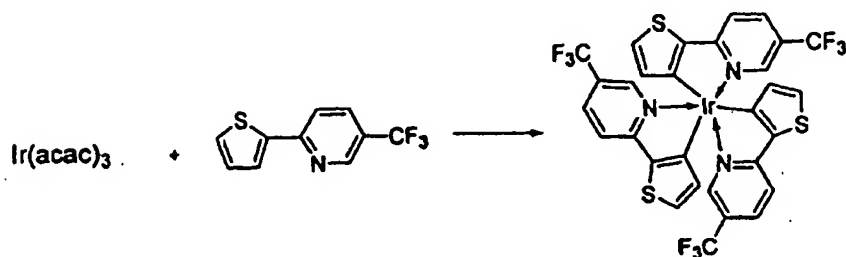
(Example 1) Synthesis of Example Compound No. 729

[0064]

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[0065] In a 100 ml-three-necked flask, 3.18 g (24.9 mmol) of thienylboronic acid, 5.65 g (25.0 mmol) of 1-bromo-4-trifluoromethylpyridine, 25 ml of toluene, 12.5 ml of ethanol and 25 ml of 2M-sodium carbonate aqueous solution, were placed and stirred at room temperature under a nitrogen stream, followed by addition of 0.98 g (0.85 mmol) of tetrakis(triphenylphosphine)palladium (0). Thereafter, the system was refluxed under stirring and nitrogen stream for 8 hours. After completion of the reaction, the reaction product was cooled and extracted by adding cold water and toluene. The organic layer was washed with saline water and dried on magnesium sulfate, followed by removal of the solvent under a reduced pressure to provide dry solid. The residue was purified by silica gel column chromatography (eluent: chloroform/methanol = 10/1) to obtain 4.20 g (yield = 74 %) of Compound A.

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[0066] In a 100 ml-four-necked flask, 50 ml of glycerol was placed and heated for 2 hours at 130 - 140 °C under stirring and bubbling with nitrogen. The glycerol was cooled to room temperature and poured into 300 ml of 1N-hydrochloric acid, and the precipitate was filtered out and washed with water. The precipitate was then purified by silica gel chromatography with chloroform as eluent, to obtain 0.33 g (yield: 38 %) of red powdery Example Compound No. 729.

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[0067] A toluene solution of the compound exhibited a luminescence spectrum showing $\lambda_{\text{max}} = 563$ nm. The compound was subjected to MALDI-TOF (matrix-assisted laser desorption ionization time-of-flight mass spectroscopy) by using an apparatus ("REFLEX-III", made by Bruker Co.). In the method, an ion obtained by removing one electron from a sample substance is subjected to measurement of a mass thereof, so that the measured mass is denoted by M^+ , and the method is frequently used for identification of a substance. The measured M^+ value was 877.0 from which the objective product was confirmed.

[0068] For confirmation of phosphorescence-type luminescence, the Example Compound was dissolved in chloroform, and the solution was separately aerated with oxygen or nitrogen, each followed by photoirradiation for comparison of photoluminescence. As a result, substantially no luminescence attributable to the iridium complex was recognized with respect to the oxygen-aerated solution, whereas photoluminescence was confirmed with respect to the nitrogen-aerated solution. From these results, the compound of the present invention was confirmed to be a phosphorescent compound. For reference, in the case of a fluorescent material, luminescence attributable to the compound does not disappear even in an oxygen-aerated solution.

[0069] Further, in contrast with a fluorescent material generally showing a luminescence life of several nsec to several tens of nsec, the compounds of the present invention including those obtained in the following Examples, all exhibited a phosphorescence life of 100 nsec or longer.

(Example 2)

[0070] Example Compound No. 310 was synthesized through a similar process as in Example 1.

Luminescence of toluene solution: $\lambda_{\text{max}} = 489$ nm

MALDI-TOF MS: $M^+ = 859.1$

(Example 3)

[0071] Example Compound No. 238 was synthesized through a similar process as in Example 1.

Luminescence of toluene solution: $\lambda_{\text{max}} = 515$ nm

MALDI-TOF MS: $M^+ = 709.1$

(Example 4)

[0072] Example Compound No. 242 was synthesized through a similar process as in Example 1.

Luminescence of toluene solution: $\lambda_{\text{max}} = 471$ nm

MALDI-TOF MS: $M^+ = 763.1$

(Example 5)

[0073] Example Compound No. 384 was synthesized through a similar process as in Example 1.

Luminescence of toluene solution: $\lambda_{\text{max}} = 466$ nm

MALDI-TOF MS: $M^+ = 913.1$

(Example 6)

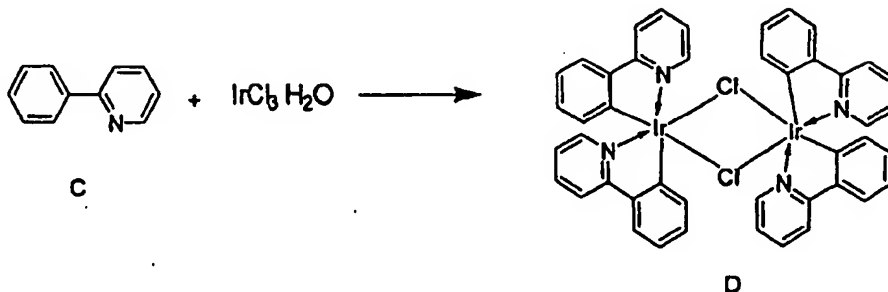
[0074] Example Compound No. 777 was synthesized through a similar process as in Example 1.

Luminescence of toluene solution: max = 696 nm

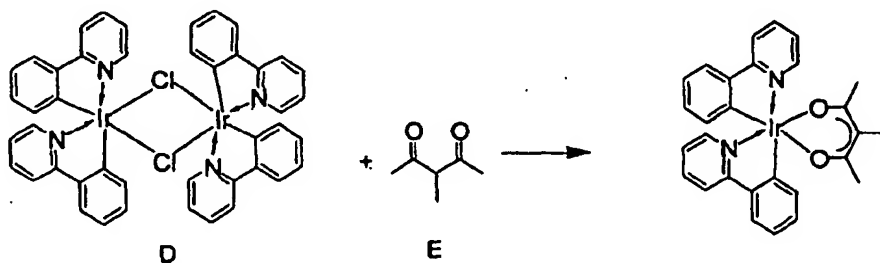
MALDI-TOF MS: $M^+ = 1231.1$

(Example 7)

[0075] Example Compound No. 472 was synthesized.



[0076] In a 100 ml-two-necked flask, 60 ml of ethoxyethanol and 20 ml of H₂O were placed and stirred for 1 hour under bubbling with nitrogen. Then, .51 g (4.4 mmol) of Compound C and 0.71 g (2.0 mmol) of iridium (III) trichloride hydrate were added, and the system was heated for 16 hours around 100 °C under stirring and nitrogen stream. The reaction product was cooled to room temperature and poured into 100 ml of water, followed by recovery by filtration and washing with water of the precipitate. The precipitate was then poured into 60 ml of ethanol and stirred for 1 hour, followed by filtering-out and washing with acetone, to obtain 0.95 g (yield: 89 %) of yellow powdery Compound D.



[0077] In a 100 ml-two-necked flask, 50 ml of ethoxyethanol was placed and stirred for 1 hour under bubbling with nitrogen. Then, 0.536 g (0.5 mmol) of Compound D, 0.17 g (1.4 mmol) of Compound E and 0.75 g of sodium carbonate Na₂CO₃ were added, and the system was heated for 16 hours around 100 °C under stirring and nitrogen stream. The reaction product was cooled to room temperature and poured into 100 ml of water, followed by filtering-out and washing with water of the precipitate. The precipitate was poured into 70 ml of ethanol, and after stirring for 1 hour, the precipitate was filtered out and dissolved in chloroform, followed by filtration. The resultant filtrate was condensed, and purified by silica gel column chromatography with chloroform as eluent to obtain 0.45 g (yield: 73 %) of yellow powdery Example Compound No. 472. A toluene solution of the compound exhibited a luminescence spectrum showing $\lambda_{\text{max}} = 526$ nm. The compound exhibited $M^+ = 614.2$ according to MALDI-TOF MS and was confirmed to be the objective product.

(Example 8)

[0078] In this Example, a device (effective display area = 3 mm²) having a device structure including 4 organic layers as shown in Figure 1(c) was prepared. An alkali-free glass sheet was used as a transparent substrate 15 and a 100 nm-thick indium tin oxide (ITO) film was formed by sputtering and patterned as a transparent electrode 14. Further, α -NPD represented by the above-mentioned structural formula was vacuum-deposited in a layer thickness of 40 nm thereon as a hole-transporting layer 13. Then, as an organic luminescence layer 12, the above-mentioned CBP as a host material and Example Compound No. 729 (metal coordination compound) in an amount of providing 8 wt. % were co-vacuum deposited in a layer thickness of 30 nm. Further, as an exciton diffusion-prevention layer 17, BCP was vacuum-deposited in a thickness of 10 nm. Then, as an electron-transporting layer 16, the above-mentioned Alq3 was subjected to resistance heating vacuum deposition at a vacuum of 10⁻⁴ Pa to form an organic film in a thickness of 30 nm.

[0079] On the above, as a lower layer of a metal electrode layer 11, an AlLi alloy film was disposed in a thickness of 15 nm, and a 100 nm-thick Al film was vacuum-deposited thereon to form a patterned metal electrode 11 disposed opposite to the transparent electrode 14 and having an electrode area of 3 mm².

[0080] The performances of the thus-obtained EL device were measured by using a micro-current meter ("4140B", made by Hewlett-Packard Corp.) for a current-voltage characteristic and "BM7" (made by Topcon K.K.) for an emission luminance.

(Example 9)

[0081] A device was prepared in the same manner as in Example 8 except using a metal coordination compound (Example Compound No. 729) was used in a weight ratio of 7 wt. %.

(Comparative Example 1)

[0082] A device was prepared in the same manner as in Example 8 except for using a metal coordination compound (729R) shown in Table 2 (wherein a substituted compound of the present invention to be compared therewith is shown in parallel) in a weight ratio of 8 wt. %.

Table 2

No	M	N	m	A	B	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	B-R7	B-R8
729R	Ir	3	0	Tn1	P1	H	H	-	-	H	H	H	H
729	Ir	3	0	Tn1	P1	H	H	-	-	H	H	CF ₃	H

(Comparative Example 2)

[0083] A device was prepared in the same manner as in Example 8 except for using the metal coordination compound (729R) shown in Table 2 in a weight ratio of 3 wt. %.

(Comparative Example 3)

[0084] A device was prepared in the same manner as in Example 8 except for using the metal coordination compound (729R) shown in Table 2 in a weight ratio of 1 wt. %.

[0085] Each device was supplied with an electric field of 12 volts/100 nm with the ITO side as the anode and the Al side as the cathode to measure a luminance.

[0086] In order to remove factors for device deterioration due to oxygen or water, the above-measurement was performed in a dry nitrogen flow after taking the device out of the vacuum chamber.

[0087] The results of devices using the respective compounds are shown in Table 3. As is understood from the results shown in Table 3, the maximum luminance concentration of Comparative Compound 729R was clearly between 1 % and 8 %, whereas Example Compound No. 729 provided with a substituent exhibited a higher luminance at 8 % than at 7 % and could exhibit a substantially higher luminance at 8 % than 729R having no substituent.

Table 3

<Luminance comparison>			
Example	Compound No.	Concentration (wt.%)	Luminance (cd/m ²)
8	729	8	4500
9	729	7	4250
Comp. 1	729R	8	1620
Comp. 2	729R	3	4000
Comp. 3	729R	1	1290

(Example 10)

[0088] A device was prepared in the same manner as in Example 8 except for using a metal coordination compound (310) synthesized in Example 2 in a weight ratio of 3 wt. %.

(Example 11)

[0089] A device was prepared in the same manner as in Example 8 except for using a metal coordination compound (310) synthesized in Example 2 in a weight ratio of 6 wt. %.

(Example 12)

[0090] A device was prepared in the same manner as in Example 8 except for using a metal coordination compound (310) synthesized in Example 2 in a weight ratio of 8 wt. %.

(Example 13)

[0091] A device was prepared in the same manner as in Example 8 except for using a metal coordination compound (238) synthesized in Example 3 in a weight ratio of 3 wt. %.

(Example 14)

[0092] A device was prepared in the same manner as in Example 8 except for using a metal coordination compound (238) synthesized in Example 3 in a weight ratio of 6 wt. %.

(Example 15)

[0093] A device was prepared in the same manner as in Example 8 except for using a metal coordination compound (238) synthesized in Example 3 in a weight ratio of 8 wt. %.

(Example 15A)

[0094] A device was prepared in the same manner as in Example 8 except for using a metal coordination compound (238) synthesized in Example 3 in a weight ratio of 11 wt. %.

(Example 15B)

[0095] A device was prepared in the same manner as in Example 8 except for using a metal coordination compound (238) synthesized in Example 3 in a weight ratio of 13 wt. %.

(Example 16)

[0096] A device was prepared in the same manner as in Example 8 except for using a metal coordination compound (242) synthesized in Example 4 in a weight ratio of 3 wt. %.

(Example 17)

[0097] A device was prepared in the same manner as in Example 8 except for using a metal coordination compound (242) synthesized in Example 4 in a weight ratio of 6 wt. %.

(Example 18)

[0098] A device was prepared in the same manner as in Example 8 except for using a metal coordination compound (242) synthesized in Example 4 in a weight ratio of 8 wt. %.

(Example 19)

[0099] A device was prepared in the same manner as in Example 8 except for using a metal coordination compound (384) synthesized in Example 5 in a weight ratio of 3 wt. %.

(Example 20)

[0100] A device was prepared in the same manner as in Example 8 except for using a metal coordination compound (384) synthesized in Example 5 in a weight ratio of 6 wt. %.

(Example 21)

[0101] A device was prepared in the same manner as in Example 8 except for using a metal coordination compound (384) synthesized in Example 5 in a weight ratio of 8 wt. %.

(Comparative Example 4)

[0102] A device was prepared in the same manner as in Example 8 except for using a metal coordination compound (1R) shown in Table 4 (wherein structures of the corresponding Example Compound Nos. 310, 238, 242 and 384 are shown in parallel) in a weight ratio of 3 wt. %.

Table 4

No	M	m	n	A	B	A-R1	A-R2	A-R3	A-R4	B-R5	B-R6	3-R7	B-R8
1R	Ir	3	0	Ph	P1	H	H	H	H	H	H	H	H
310	Ir	3	0	Ph	P1	H	CF ₃	H	H	H	H	H	H
238	Ir	3	0	Ph	P1	H	F	H	H	H	H	H	H
242	Ir	3	0	Ph	P1	F	H	F	H	H	H	H	H
384	Ir	3	0	Ph	P1	H	CF ₃	F	H	H	H	H	H

(Comparative Example 5)

[0103] A device was prepared in the same manner as in Example 8 except for using the metal coordination compound (1R) shown in Table 4 in a weight ratio of 6 wt. %.

(Comparative Example 6)

[0104] A device was prepared in the same manner as in Example 8 except for using the metal coordination compound (1R) shown in Table 4 in a weight ratio of 8 wt. %.

[0105] Each device of Examples 10 - 12 and Comparative Examples 4 - 6 was supplied with an electric field of 12 volts/100 nm with the ITO side as the anode and the Al side as the cathode to measure a current efficiency.

[0106] The results of devices using the respective compounds are shown in Table 5. As is understood from the results shown in Table 5, the concentration giving a maximum current efficiency of Comparative Compound 1R was clearly between 3 % and 8 %, whereas Example Compound No. 310 provided with a substituent exhibited an increase in current efficiency even at 8 %.

Table 5

<Comparison of current efficiency>			
Example	Compound No.	Concentration (wt.%)	Current Eff. (cd/A)
10	310	3	2
11	310	6	2.4
12	310	8	2.7
Comp. 4	1R	3	15
Comp. 5	1R	6	19
Comp. 6	1R	8	17

[0107] Each device of Examples 13 - 15 and Comparative Examples 4 - 6 was supplied with a voltage of 12 volts/ 100 nm with the ITO side as the anode and the Al side as the cathode to measure an (electric) power efficiency.

[0108] The results of the devices using the respective compounds are shown in Table 6. As is understood from the results shown in Table 6, the concentration giving a maximum power efficiency of the Comparative Compound 1R was between 3 % and 8 %, whereas Example Compound (238) provided with a substituent showed an increase in maximum efficiency even at a concentration of 8 %.

Table 6

<Comparison of power efficiency>			
Example	Compound No.	Concentration (wt.%)	Power efficiency (lm/W)
13	238	3	5.4
14	238	6	6
15	238	8	6.2
15A	238	11	6.5
15B	238	13	6.3
Comp. 4	1R	3	5.7
Comp. 5	1R	6	6.2
Comp. 6	1R	8	6

[0109] Each device of Examples 16 - 18 and Comparative Examples 4 - 6 was supplied with a voltage of 12 volts/ 100 nm with the ITO side as the anode and the Al side as the cathode to measure an external quantum efficiency, which was evaluated in terms of a ratio of luminance (lm)/current (mA) based on a value of current passing through the device by using a micro-current passing through the device by using a micro-current meter ("4140B", made by Hewlett-Packard Corp.) and a value of luminance measured by "BM7" (made by Topcon K.K.).

[0110] The results of the devices using the respective compounds are shown in Table 7. As is understood from the results shown in Table 7, the concentration giving a maximum external quantum efficiency of the Comparative Compound 1R was between 3 % and 8 %, whereas Example Compound (242) provided with a substituent showed an increase in maximum efficiency even at a concentration of 8 %.

Table 7

<Comparison of external quantum efficiency>			
Example	Compound No.	Concentration (wt.%)	Ext. quantum efficiency
16	242	3	3
17	242	6	4
18	242	8	4.2
Comp. 4	1R	3	7
Comp. 5	1R	6	8
Comp. 6	1R	8	7.6

[0111] Each device of Examples 19 - 21 and Comparative Examples 4 - 6 was supplied with a voltage of 12 volts/ 100 nm with the ITO side as the anode and the Al side as the cathode to measure an (electric) power efficiency.

[0112] The results of the devices using the respective compounds are shown in Table 8. As is understood from the results shown in Table 8, the concentration giving a maximum power efficiency of the Comparative Compound 1R was between 3 % and 8 %, whereas Example Compound (384) provided with a substituent showed an increase in maximum efficiency even at a concentration of 8 %.

Table 8

<Comparison of power efficiency>			
Example	Compound No.	Concentration (wt.%)	Power efficiency (lm/W)
19	384	3	2
20	384	6	2.3
21	384	8	2.6
Comp. 4	1R	3	5.7
Comp. 5	1R	6	6.2
Comp. 6	1R	8	6

(Example 22)

[0113] A device was prepared in the same manner as in Example 8 except for using a metal coordination compound (777) synthesized in Example 6 in a weight ratio of 1 wt. %.

(Example 23)

[0114] A device was prepared in the same manner as in Example 8 except for using a metal coordination compound (777) synthesized in Example 6 in a weight ratio of 6 wt. %.

(Example 24)

[0115] A device was prepared in the same manner as in Example 8 except for using a metal coordination compound (777) synthesized in Example 6 in a weight ratio of 8 wt. %.

(Comparative Example 7)

[0116] A device was prepared in the same manner as in Example 8 except for using a metal coordination compound (777R) shown in Table 9 below in a weight ratio of 1 wt. %.

Table 9

No	M	m	n	A	B	A-R1	A-R2	A-R3	A-R4	3-R5	3-R6	B-R7	B-R8
777R	Ir	3	0	Pe	P1	H	H	H	H	H	H	H	H
777	Ir	3	0	Pe	P1	H	H	H	H	H	H	CF ₃	H

(Comparative Example 8)

[0117] A device was prepared in the same manner as in Example 8 except for using the metal coordination compound (777R) shown in Table 9 in a weight ratio of 6 wt. %.

(Comparative Example 9)

[0118] A device was prepared in the same manner as in Example 8 except for using the metal coordination compound (777R) shown in Table 9 in a weight ratio of 8 wt. %.

[0119] Each device of Examples 22 - 25 and Comparative Examples 7 - 9 was supplied with a voltage of 12 volts/ 100 nm with the ITO side as the anode and the Al side as the cathode to measure an (electric) power efficiency.

[0120] The results of the devices using the respective compounds are shown in Table 10. As is understood from the results shown in Table 6, the concentration giving a maximum power efficiency of Comparative Compound 777R was between 1 % and 8 %, whereas Example Compound (777) provided with a substituent showed an increase in maximum

efficiency up to a concentration of 8 %.

Table 10

<Comparison of maximum power efficiency>			
Example	Compound No.	Concentration (wt.%)	Power efficiency (lm/W)
22	777	1	0.04
23	777	6	0.12
24	777	8	0.15
Comp. 7	777R	1	0.08
Comp. 8	777R	6	0.15
Comp. 9	777R	8	0.13

(Example 25)

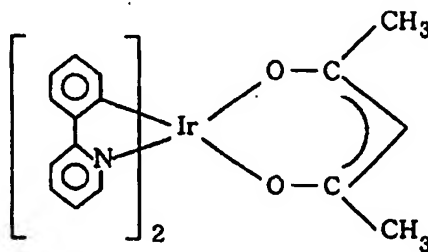
[0121] A device was prepared in the same manner as in Example 8 except for using a metal coordination compound (472) synthesized in Example 7 in a weight ratio of 3 wt. %.

(Example 26)

[0122] A device was prepared in the same manner as in Example 1 except for using a metal coordination compound (472) synthesized in Example 7 in a weight ratio of 6 wt. %.

(Comparative Example 10)

[0123] A device was prepared in the same manner as in Example 1 except for using a metal coordination compound (472R) shown below in a weight ratio of 3 wt. %.



(Comparative Example 11)

[0124] A device was prepared in the same manner as in Example 1 except for using the above metal coordination compound (472R) in a weight ratio of 6 wt. %.

(Comparative Example 12)

[0125] A device was prepared in the same manner as in Example 1 except for using the above metal coordination compound (472R) in a weight ratio of 8 wt. %.

[0126] Each device of Examples 25 - 27 and Comparative Examples 10 - 12 was supplied with an electric field of 12 volts/100 nm with the ITO side as the anode and the Al side as the cathode to measure a power efficiency.

[0127] In order to remove factors for device deterioration due to oxygen or water, the above-measurement was performed in a dry nitrogen flow after taking the device out of the vacuum chamber.

[0128] The results of devices using the respective compounds are shown in Table 11. As is understood from the results shown in Table 11, the concentration giving a maximum power efficiency of Comparative Compound 1R was clearly between 3 % and 8 %, whereas Example Compound (384) provided with a substituent exhibited an increase in power efficiency even at a concentration of 8 %.

Table 11

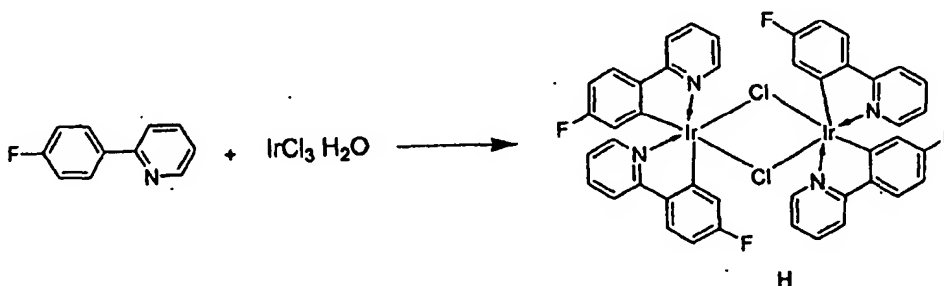
<Comparison of maximum power efficiency>			
Example	No.	Concentration (wt.%)	Power efficiency (1m/W)
25	472	3	5.6
26	472	6	6.3
27	472	8	6.5
Comp. 10	472R	3	5.4
Comp. 11	472R	6	6
Comp. 12	472R	8	5.8

(Example 28)

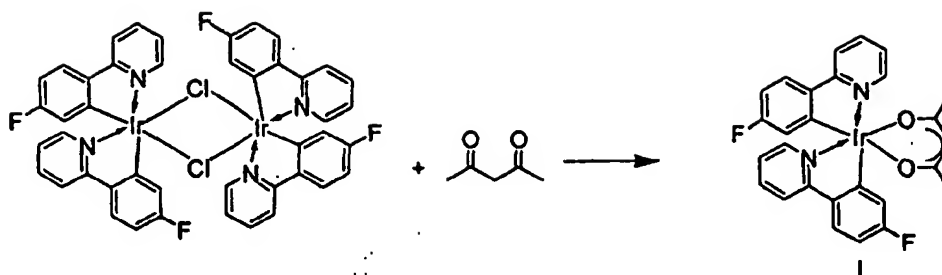
[0129]



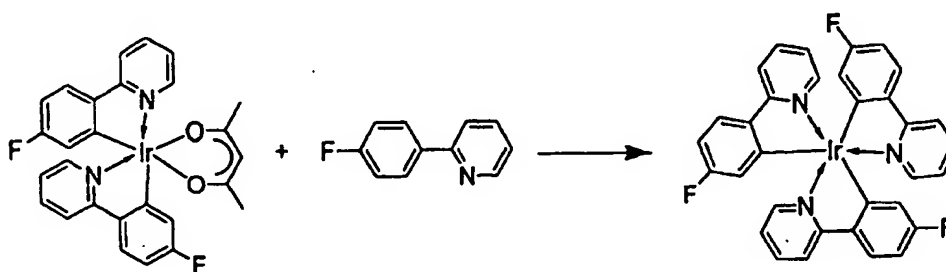
[0130] In a 200 ml-three-necked flask, 3.50 g (25.0 mmol) of 4-fluorophenylboronic acid, 3.95 g (25.0 mmol) of 1-bromopyridine, 25 ml of toluene, 12.5 ml of ethanol and 25 ml of 2M-sodium carbonate aqueous solution, were placed and stirred at room temperature under a nitrogen stream, followed by addition of 0.98 g (0.85 mmol) of tetrakis(triphenylphosphine)palladium (0). Thereafter, the system was refluxed under stirring and nitrogen stream for 8 hours. After completion of the reaction, the reaction product was cooled and extracted by adding cold water and toluene. The organic layer was washed with saline water and dried on magnesium sulfate, followed by removal of the solvent under a reduced pressure to provide dry solid. The residue was purified by silica gel column chromatography (eluent: chloroform/methanol = 10/1) to obtain 3.24 g (yield = 75 %) of Compound G.



[0131] In a 200 ml-three-necked, 0.881 g (2.5 mmol) of iridium (III) chloride trihydrate, 0.953 g (5.5 mmol), 75 ml of ethoxyethanol and 25 ml of water were placed and stirred for 30 min. at room temperature under nitrogen stream, followed by 24 hours of reflux under stirring. The reaction product was cooled to room temperature, and the precipitate was recovered by precipitation and washed successively with water, ethanol and acetone. After being dried at room temperature under a reduced pressure, 1.32 g (yield: 92 %) of yellow powdery Compound H was obtained.



[0132] In a 200 ml-three-necked flask, 70 ml of ethoxyethanol, 0.80 g (0.7 mmol) of Compound H, 0.22 g (2.10 mmol) of acetylacetone and 1.04 g (9.91 mmol) of sodium carbonate, were placed and stirred for 1 hour at room temperature under a nitrogen stream, followed by 15 hours of reflux under stirring. The reaction product was cooled with ice, and the precipitate was filtered out and washed with water. The precipitate was purified by silica gel chromatography (eluent: chloroform/methanol = 30/1) to obtain 0.63 g (yield: 71 %) of yellow powdery Compound I (Example Compound No. 489). A toluene solution of the compound exhibited a luminescence spectrum showing $\lambda_{\text{max}} = 499$ nm. Further, according to MALDI-TOF MS, $M^+ = 638.7$ of the compound was confirmed.



[0133] In a 100 ml-three-necked flask, 0.21 g (1.2 mmol) of Compound G, 0.32 g (0.5 mmol) of Compound I and 25 ml of glycerol, were placed and stirred for 8 hours around 180 °C under a nitrogen stream. The reaction product was cooled to room temperature and poured into 170 ml of 1N-hydrochloric acid. The precipitate was filtered out and washed with water, followed by drying for 5 hours at 100 °C under a reduced pressure. The precipitate was purified by silica gel column chromatography with chloroform as the eluent to obtain 0.22 g (yield: 63 %) of yellow powdery Example Compound No. 239. A toluene solution of the compound exhibited a luminescence spectrum showing $\lambda_{\text{max}} = 490$ nm, and $M^+ = 708.8$ of the compound was confirmed by MALDI-TOF MS.

(Example 29)

[0134] Example Compound No. 535 was synthesized through a similar process as in Example 7.

Luminescence of toluene solution: $\lambda_{\text{max}} = 525$ nm

MALDI-TOF MS: $M^+ = 671.1$

(Example 30)

[0135] Example Compound No. 243 was synthesized through a similar process as in Example 28.

Luminescence of toluene solution: $\lambda_{\text{max}} = 518$ nm

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MALDI-TOF MS: $M^+ = 762.7$

(Example 31)

[0136] Example Compound No. 511 was synthesized through a similar process as in Example 7.

Luminescence of toluene solution: $\lambda_{\max} = 514$ nm

MALDI-TOF MS: $M^+ = 628.1$

(Example 32)

[0137] Example Compound No. 56 was synthesized through a similar process as in Example 28.

Luminescence of toluene solution: $\lambda_{\max} = 505$ nm

MALDI-TOF MS: $M^+ = 697.2$

(Example 33)

[0138] Example Compound No. 389 was synthesized through a similar process as in Example 1.

Luminescence of toluene solution: $\lambda_{\max} = 503$ nm

(Example 34)

[0139] Example Compound No. 390 was synthesized through a similar process as in Example 1.

Luminescence of toluene solution: $\lambda_{\max} = 507$ nm

(Example 35)

[0140] Example Compound No. 312 was synthesized through a similar process as in Example 1.

[0141] The Luminescence of toluene solution exhibited two peaks at 458 nm and 488 nm.

(Example 36)

[0142] Example Compound No. 312 is synthesized through a similar process as in Example 1.

(Example 37)

[0143] Example Compound No. 314 is synthesized through a similar process as in Example 1.

(Example 38)

[0144] Example Compound No. 388 is synthesized through a similar process as in Example 1.

(Example 39)

[0145] Example Compound No. 392 is synthesized through a similar process as in Example 1.

(Example 40)

[0146] Example Compound Nos. 274, 346, 358, 393 and 396 can be synthesized through a similar process except for changing the starting material.

(Example 41)

[0147] Hereinbelow, two examples of display apparatus are described. First, an example of preparation of a picture display apparatus having an XY-matrix structure is described with reference to Figure 2.

[0148] On a glass substrate 21 measuring 150 mm-length, 150 mm-width and 1.1 mm-thickness, a ca. 100 nm-thick ITO film was formed by sputtering and patterned into 100 lines of 100 μm -wide transparent matrix electrodes (anode side) with a spacing of 40 μm as simple matrix electrodes. Then, a four-layered organic compound layer 23 was formed thereon including a luminescence layer 12 containing one of the compounds synthesized in Examples 1 - 7 as a guest compound.

[0149] Then, 100 lines of 100 μm -wide metal electrodes 24 were formed with a spacing of 40 μm by mask vacuum deposition so as to be perpendicular to the transparent electrodes by vacuum deposition at a vacuum of 2×10^{-5} Torr. The metal electrodes were formed as a lamination of 10 nm-thick layer of Al/Li alloy (Li: 1.3 wt. %) and then 150 nm-thick layer of A1.

[0150] The thus-obtained 100x100-simple matrix-type organic EL devices were subjected to a simple matrix drive in a glove box filled with nitrogen at voltages of 7 volts to 13 volts by using a scanning signal of 10 volts and data signals of ± 3 volts as shown in Figure 3. As a result of an interlaced drive at a frame frequency of 30 Hz, luminescence pictures were confirmed for the respective devices.

[0151] As a picture display apparatus, the high-efficiency luminescence device of the present invention allows a light-weight flat panel display with economized energy consumption and high-recognizability. As a printer light source, the luminescence devices of the present invention may be arranged in a line and disposed in proximity to the photosensitive drum, to provide a line shutter wherein the respective devices are driven independently from each other to effect prescribed exposure on the photosensitive drum. On the other hand, the energy consumption economization effect is expected in application as an illumination device or a backlight for a liquid crystal display apparatus.

[0152] For another application to a picture display device, it is particularly advantageous to form an active matrix-type picture display device equipped with thin film transistors (TFTs) instead of the above-mentioned XY-matrix wiring. Hereinbelow, an active matrix-type picture display device according to the present invention will be described with reference to Figures 4 to 6.

[0153] Figure 4 is a schematic plan view of such a panel. Circumferentially outside the panel are disposed a drive circuit comprising a power supply source and a scanning signal driver, and a data signal driver as a display signal input means (called a picture data supply means, which are respectively connected to current supply lines, X-direction scanning lines called gate lines and Y-direction lines called data lines. The scanning signal driver sequentially selects the gate scanning lines, and in synchronism therewith, picture signals are supplied from the data signal driver. Display pixels are disposed at intersections of the gate scanning lines and the data lines.

[0154] Next, a pixel circuit operation is described with reference to an equivalent circuit. When a selection signal is applied to a gate selection line, TFT1 is turned on so that a data signal is supplied from a data signal line to a capacitor Cadd, thereby determining the gate potential of TFT2, whereby a current is supplied to an organic luminescence device (EL) disposed at each pixel through a current supply line depending on the gate potential of TFT2. The gate potential of TFT2 is held at Cadd during one frame period, so that the current continually flows from the current supply line to the EL device during the period. As a result, luminescence is retained during one frame period.

[0155] Figure 6 is a schematic view illustrating a sectional structure of a TFT used in this Example. On a glass substrate, a polysilicon p-Si layer is formed, and the channel, drain and source regions are doped with necessary impurities, respectively. Thereon, gate electrodes are formed via a gate insulating film, and drain electrodes and source electrodes connected to the drain regions and source regions, respectively, are formed. In this instance, the drain electrodes and transparent pixel electrodes (ITO) are connected through contact holes bored in an intervening insulating film.

[0156] The active device used in the present invention need not be particularly restricted, and can also be a single-crystal silicon TFT, an amorphous silicon a-Si TFT, etc.

[0157] On the pixel electrodes, plural layers or a single layer of organic luminescence layer may be disposed and metal electrodes as cathode are sequentially laminated to provide an active-type organic luminescence device.

[INDUSTRIAL APPLICABILITY]

[0158] As described above, a substituted metal coordination compound having a high phosphorescence efficiency

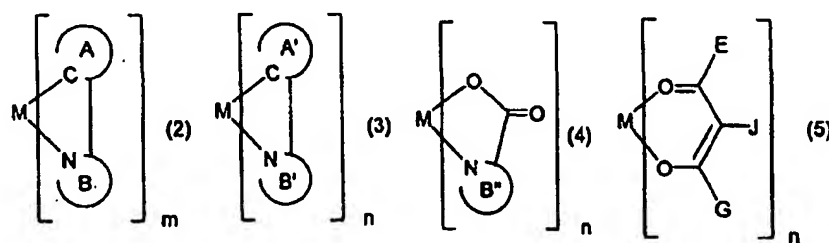
and a short phosphorescence life can be used in a luminescence layer at a high concentration relative to the host material while preventing concentration extinction. As a result, according to the present invention, it is possible to obtain an excellent luminescence device showing high luminescence efficiency. The luminescence device of the present invention is also excellent as a display device.

Claims

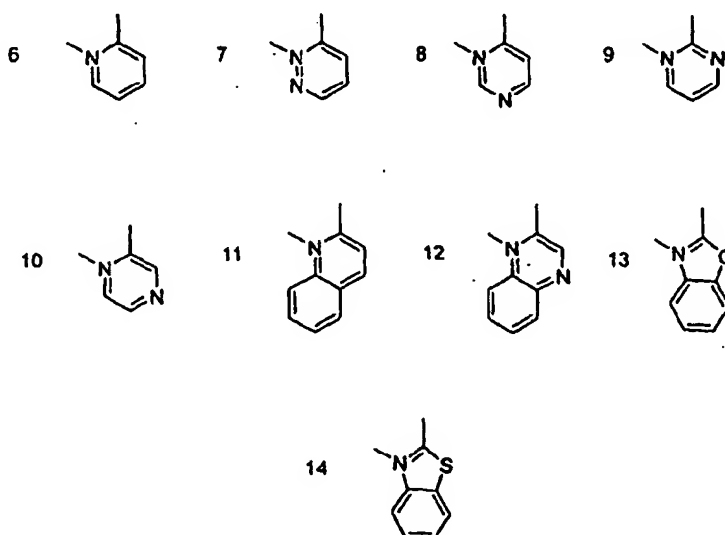
1. An organic luminescence device, comprising: a pair of electrodes each disposed on a substrate, and at least one luminescence layer comprising an organic compound disposed between the electrodes; wherein the luminescence layer comprises a non-luminescent first organic compound and a phosphorescent second organic compound represented by formula (1) shown below, and the second organic compound is present at a concentration of at least 8 wt. % in the luminescence layer:



wherein M is a metal atom of Ir, Pt, Rh or Pd; L and L' are mutually different bidentate ligands; m is 1, 2 or 3; n is 0, 1 or 2 with the proviso that m+n is 2 or 3; a partial structure ML_m is represented by formula (2) shown below and a partial structure ML'_n is represented by formula (3), (4) or (5) shown below:



wherein N and C are nitrogen and carbon atoms, respectively; A and A' are respectively a cyclic group capable of having a substituent and bonded to the metal atom M via the carbon atom; B, B' and B'' are respectively a cyclic group represented by a formula of (6) - (14) shown below capable of having a substituent and connected to the metal atom M via the nitrogen atom:



{wherein the substituent is selected from a halogen atom, a cyano group, a nitro group, a trialkylsilyl group (of which the alkyl groups are independently a linear or branched alkyl group having 1 to 8 carbon atoms), a linear or branched alkyl group having 1 to 20 carbon atoms (of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH- or -C≡C- and the alkyl group can include a hydrogen atom that can be replaced with a fluorine atom), or an aromatic cyclic group capable of having a substituent (of which the substituent is selected from a halogen atom, a cyano group, a nitro group, a linear or branched alkyl group having 1 to 20 carbon atoms (of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH- or -C≡C- and the alkyl group can include a hydrogen atom that can be replaced with a fluorine atom));

A and B, and A' and B' are respectively bonded to each other via a covalent bond;

E and G are independently a linear or branched alkyl group having 1 to 20 carbon atoms (of which the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom), or an aromatic cyclic group capable of having a substituent (of which the substituent is selected from a halogen atom, a cyano group, a nitro group, a trialkylsilyl group (of which the alkyl groups are independently a linear or branched alkyl group having 1 to 8 carbon atoms), a linear or branched alkyl group having 1 to 20 carbon atoms (of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH- or -C≡C- and the alkyl group can include a hydrogen atom that can be replaced with a fluorine atom));

J is a hydrogen atom, a halogen atom, a linear or branched alkyl group having 1 to 20 carbon atoms (of which the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom), or an aromatic cyclic group capable of having a substituent (of which the substituent is selected from a halogen atom, a cyano group, a nitro group, a trialkylsilyl group (of which the alkyl groups are independently a linear or branched alkyl group having 1 to 8 carbon atoms), or a linear or branched alkyl group having 1 to 20 carbon atoms (of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH- or -C≡C- and the alkyl group can include a hydrogen atom that can be replaced with a fluorine atom));

wherein the compound represented by the formula (1) includes at least one cyclic group having a substituent.

2. An organic luminescence device according to Claim 1, comprising: a pair of electrodes each disposed on a substrate, and at least one luminescence layer comprising an organic compound disposed between the electrodes; wherein the luminescence layer comprises a non-luminescent first organic compound and a phosphorescent second organic compound represented by the above-mentioned formula (1), and the second organic compound is present at a concentration in the luminescence layer that is higher than a concentration at which a cyclic group represented by the formula (1) but containing no substituent in any of the cyclic groups A and A' or the cyclic groups B and B' exhibits a maximum luminescence characteristic.
3. An organic luminescence device according to Claim 1, comprising: a pair of electrodes each disposed on a substrate, and at least one luminescence layer comprising an organic compound disposed between the electrodes; wherein the luminescence layer comprises a non-luminescent first organic compound and a phosphorescent second organic compound represented by the above-mentioned formula (1), and the second organic compound is present at a prescribed concentration of at least 8 wt. % in the luminescence layer providing a maximum luminescence characteristic.
4. An organic luminescence device according to Claim 1, wherein the partial structure ML'_n in the formula (1) is represented by the formula (3).
5. An organic luminescence device according to Claim 1, wherein the partial structure ML'_n in the formula (1) is represented by the formula (4).
6. An organic luminescence device according to Claim 1, wherein the partial structure ML'_n in the formula (1) is represented by the formula (5).
7. An organic luminescence device according to Claim 1, wherein n in the formula (1) is 0.
8. An organic luminescence device according to Claim 1, wherein the substituent of the compound of the formula (1) is fluorine.
9. An organic luminescence device according to Claim 1, wherein the substituent of the compound of the formula (1)

is a trifluoromethyl group.

10. An organic luminescence device according to Claim 1, wherein the substituent of the compound of the formula (1) is an alkyl group.

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11. An organic luminescence device according to Claim 2, wherein said maximum luminescence characteristic is a maximum luminescence luminance.

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12. An organic luminescence device according to Claim 2, wherein said maximum luminescence characteristic is a maximum current.

13. An organic luminescence device according to Claim 2, wherein said maximum luminescence characteristic is an external luminescence efficiency.

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14. An organic luminescence device according to Claim 2, wherein said maximum luminescence characteristic is a ratio of luminescence flux/power consumption obtained by dividing a luminescence flux by a power consumption.

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15. An organic luminescence device according to Claim 1, wherein phosphorescence is emitted from the luminescence layer by applying a voltage between the electrodes.

16. A picture display apparatus, comprising an organic luminescence device according to Claim 1, and a drive circuit for supplying display data.

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FIG. 1

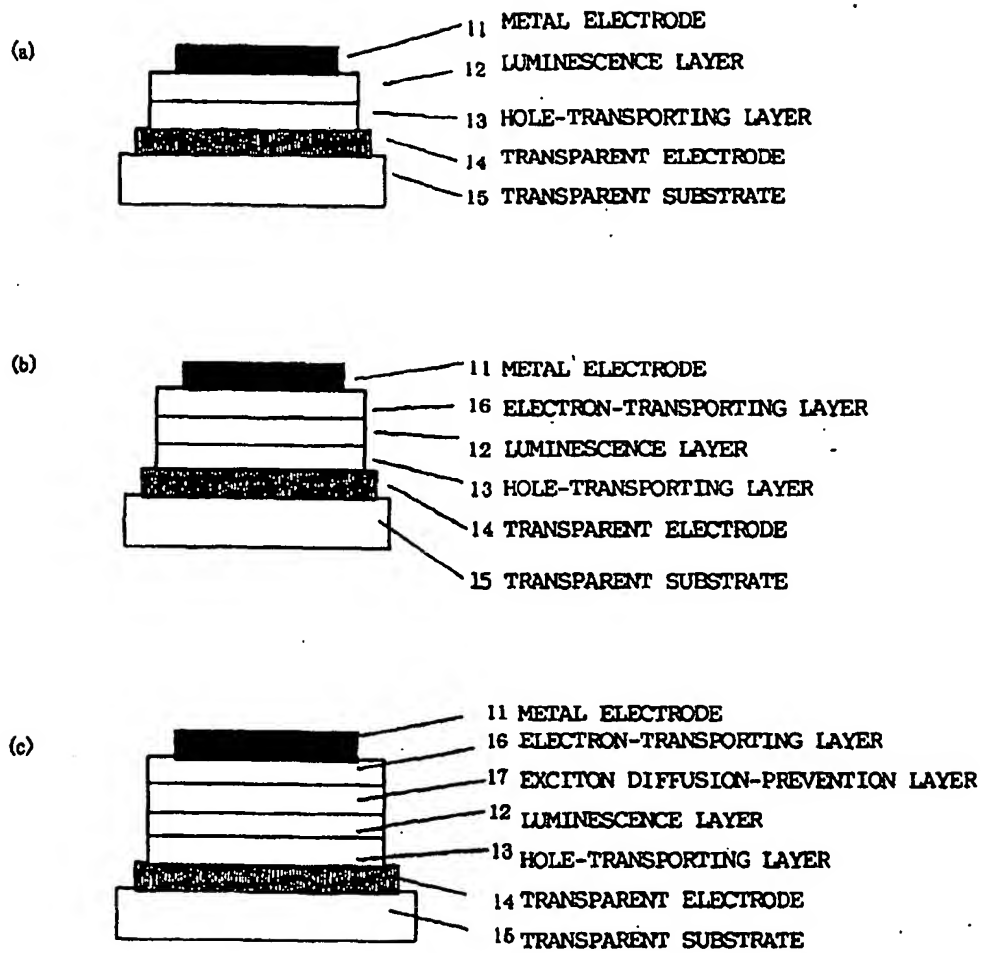


FIG. 2

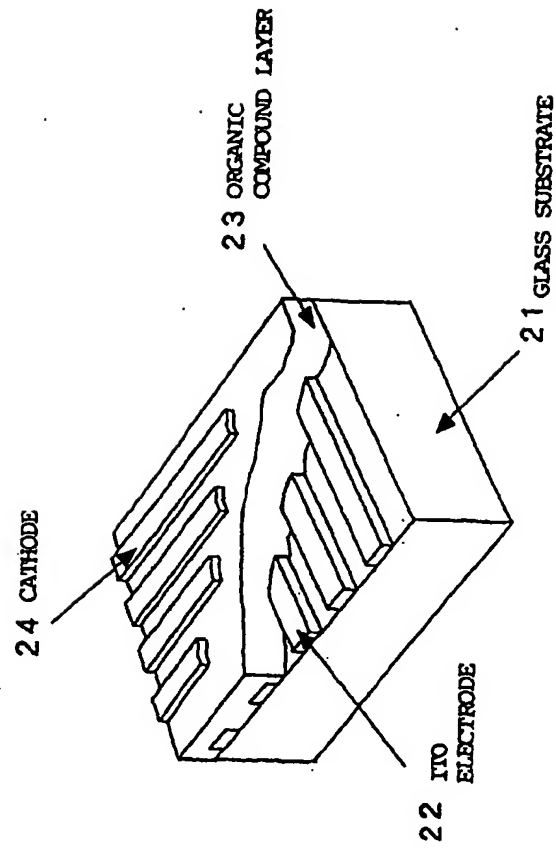


FIG. 3

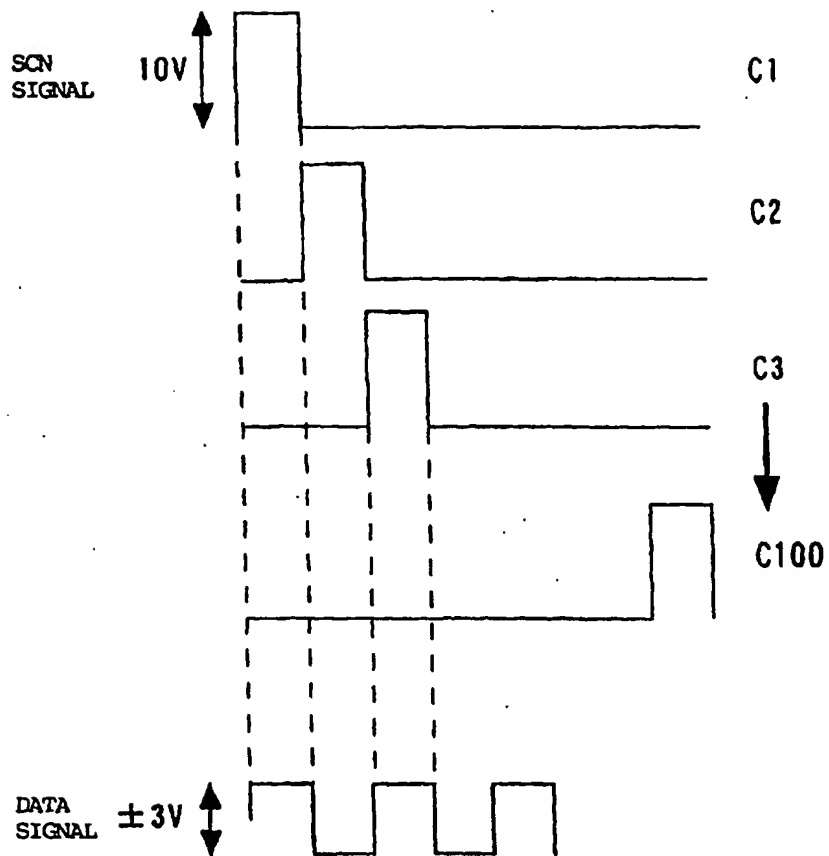


FIG. 4

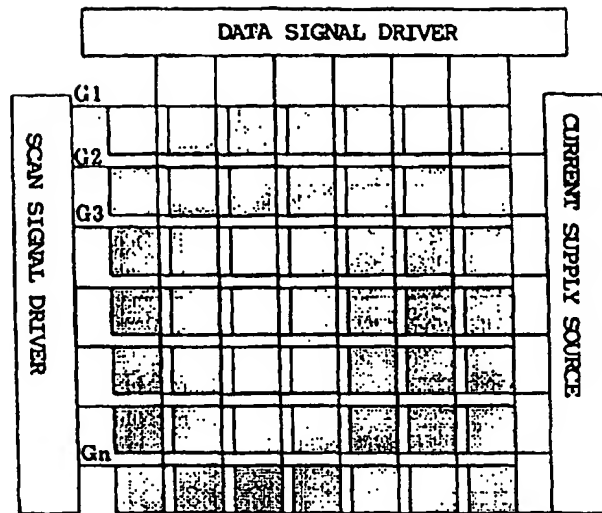


FIG. 5

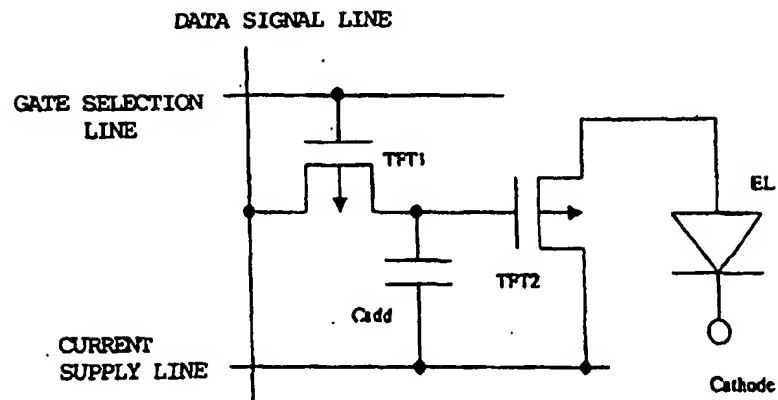
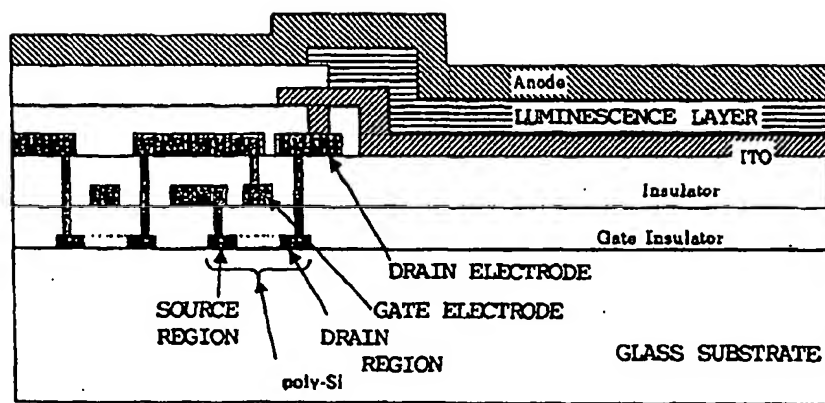


FIG. 6



INTERNATIONAL SEARCH REPORT

International application No.

PCT/JP01/10477

A. CLASSIFICATION OF SUBJECT MATTER Int.Cl. ⁷ H05B 33/14, C09K 11/06, C07F 15/00, 19/00 According to International Patent Classification (IPC) or to both national classification and IPC		
B. FIELDS SEARCHED Minimum documentation searched (classification system followed by classification symbols) Int.Cl. ⁷ H05B 33/00-33/28, C09K 11/06, C07F 15/00, 19/00 Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched Jitsuyo Shinan Koho 1922-1996 Toroku Jitsuyo Shinan Koho 1994-2002 Kokai Jitsuyo Shinan Koho 1971-2002 Jitsuyo Shinan Toroku Koho 1996-2002 Electronic data base consulted during the international search (name of data base and, where practicable, search terms used) CA (STN), JICST FILE (JOIS)		
C. DOCUMENTS CONSIDERED TO BE RELEVANT		
Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
PX	US 2001/19782 A1 (IGARASHI, Tatsuya et al.), 06 September, 2001 (06.09.2001), Full text & JP 2001-247859 A Full text & JP 2001-345183 A Full text	1, 4, 6-10, 15, 16
A	BALDO et al., "Highly Efficient Phosphorescent Emission from Organic Electroluminescent Devices", Nature, (1998), Vol.395, pages 151 to 154	1-16
A	TSUTSUI, Tetsuo et al., "High Quantum Efficiency in Organic Light-Emitting Devices with Iridium-Complex as a Triplet Emissive Center", Jpn. J. Appl. Phys., (1999), Vol.38, Part 2, No.12(B), pages L1502 to L1504	1-16
<input type="checkbox"/> Further documents are listed in the continuation of Box C. <input type="checkbox"/> See patent family annex.		
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Date of the actual completion of the international search 04 February, 2002 (04.02.02)		Date of mailing of the international search report 19 February, 2002 (19.02.02)
Name and mailing address of the ISA/ Japanese Patent Office Facsimile No.		Authorized officer Telephone No.

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